

# 1663

Atoms in a new light  
Containing nuclear contamination  
A hacker's John Hancock  
The unsung nuclear reaction



## MICROFLUIDICS

21<sup>ST</sup> CENTURY TOOL FOR  
21<sup>ST</sup> CENTURY SCIENCE





More than 100,000 stars are crammed into the globular cluster M5. Many of them (e.g., the bright reddish stars in this image) are easily identified as red giants, and inside some of the older ones, neutrons repeatedly merge with atomic nuclei to produce most of the elements on the periodic table—including a few elements that are critical to the function of the human body. See “The Other Nuclear Reaction” on page 26 for Los Alamos research on neutron-capture reactions.

*CREDIT: HST, ESA, NASA*



## About the Cover:

When fluids are manipulated in very small volumes, their behavior changes, making them more controllable than they are in larger volumes. The field of microfluidics has emerged to better characterize how fluids behave in small volumes and develop ways to apply this new understanding for the greater good. Entire laboratories are now being miniaturized and integrated onto bench-top or handheld microfluidic devices—with the cost, space, and time it takes to conduct certain types of experiments cut to a fraction of what they once were and results as good or better. Scientists at Los Alamos are working on both the science and technology of microfluidics: developing new methods of manufacturing microfluidic devices, adapting old protocols to new platforms, and generally pioneering new ways of doing things. Energy security, nuclear safeguards, biomedical research, and other science at Los Alamos all stand to benefit from this new capability.

## About Our Name:

During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

## About the LDRD Logo:

Laboratory Directed Research and Development (LDRD) is a competitive internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to national interests. Whenever 1663 reports on research that received support from LDRD, this logo appears at the end of the article.

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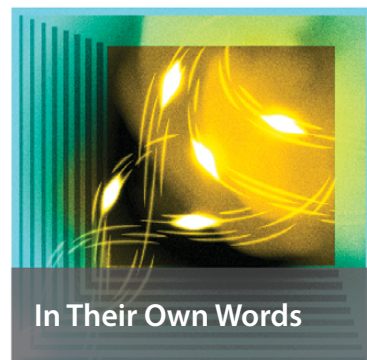


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*CREDIT: Eugene Kowaluk/University of Rochester Laboratory for Laser Energetics*

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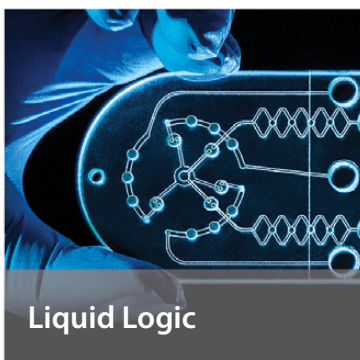
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# SPOTLIGHTS

## No Help for the Primordial Particle Soup

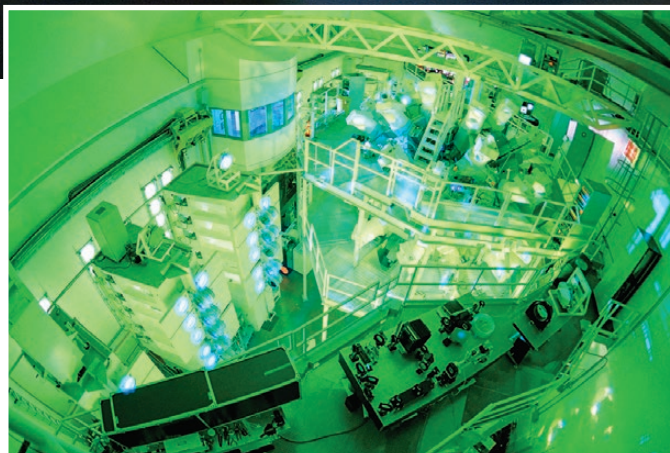
**I**N THE FIRST MINUTES OF THE BIG BANG, AS THE UNIVERSE expanded and cooled, there was a brief window when the conditions were right for the nuclear fusion of hydrogen into heavier atomic nuclei. During that episode in cosmic history, known as big bang nucleosynthesis (BBN), it was hot enough for fusion to occur but not so hot that the resulting nuclei would disintegrate. And astronomical measurements of the primordial abundances of key isotopes produced by BBN—three isotopes of hydrogen and two of helium—match the predictions of the big bang theory to exquisite precision. However, the only other element produced by BBN in any observable quantity, lithium, presents a discrepancy. For its more common isotope, lithium-7, the discrepancy is manageable, but for lithium-6, it's enormous. Observations exceed theoretical predictions by three orders of magnitude.

Alex Zylstra, a Los Alamos plasma physicist, thought he could help resolve the lithium-6 conundrum. He and others in the field knew that if a particular BBN reaction, fusing helium-3 with hydrogen-3 (also called tritium), were more active than anyone thought, it could overproduce lithium-6. And earlier measurements of that reaction rate were suspect; they were inconsistent and substantially overshoot realistic BBN conditions by relying on high-energy accelerators to produce the fusion reactions instead of lower-energy collisions between nuclei in plasma.

So Zylstra and collaborators developed a more realistic alternative, using an advanced research facility funded by the Department of Energy (DOE), the OMEGA laser at the University of Rochester's Laboratory for Laser Energetics, to heat a mixture of tritium and helium-3 to BBN-appropriate temperatures. In a pulse lasting less than a billionth of a second, sixty powerful lasers converged on the isotope mixture,

(Top) Inside the target chamber for the OMEGA laser, 60 laser beams converge on a millimeter-sized target capsule to produce an imploding, nuclear-fusion supporting plasma at a temperature of more than 200 million kelvins. (Bottom) The OMEGA target bay bathed in its own light during a target shot.

CREDIT: Eugene Kowaluk/University of Rochester Laboratory for Laser Energetics



generating a dramatic implosion to deliver the necessary heating. (Zylstra also conducts similar fusion experiments at another laser-implosion facility, the bigger and more powerful National Ignition Facility, or NIF, at Lawrence Livermore National Laboratory.)

But rather than solving the lithium-6 mystery, Zylstra's experiment ended up compounding it. The measurements convincingly showed that the reaction rate was too low to generate all the excess lithium-6, making it more likely that the troublesome isotope is synthesized elsewhere by some as-yet undiscovered process, perhaps taking place inside early stars. However, the experiment firmed up the tritium-helium-3 reaction rate, showing that it had been inaccurately reported in previously published BBN calculations. And perhaps more importantly, it demonstrated for the first time how plasma-fusion laser facilities like OMEGA and NIF, primarily developed for research supporting stewardship of the nation's nuclear-weapons arsenal, can be double-purposed to benefit nuclear astrophysics research as well. **LDRD**

—Craig Tyler



## Beating the Best Camouflage

**T**HE ABILITY TO BLEND IN IS VERY USEFUL IN THE ANIMAL kingdom, where every day is an adventure in the rule of eat or be eaten. Animals from all walks of life have developed elaborate mechanisms of camouflage that seem to have evolved to foil the exact cues upon which animal and human vision rely most heavily—color, texture, and edges.

The excellent blending abilities of some animals pose challenges for marine biologists and oceanographers in knowing where, and how abundant, these animals are. Flounder fish are a bellwether fauna for ocean health, so it's important for scientists to have accurate population data. But because they are also masters of disguise—able to change their coloration to imitate the color and texture of the ocean floor—flounder can be hard to find.

Human eyes are better at finding hidden objects in photographs than today's computers are. But doing so is an incredibly tedious task with a high rate of burnout, because fatigued eyes can fail. Computers can work around the clock without getting tired, but they just aren't that good at the task. Los Alamos data scientist Lakshman Prasad is working to change that. By studying how and why human vision fails to find hidden things, and what cues get missed, Prasad is figuring out how to train computers to reliably spot animals that are trying to hide. In a collaboration with Woods Hole Oceanographic Institute and the National Oceanic and Atmospheric Administration, Prasad has developed an algorithm that automatically analyzes images of the seafloor for tell-tale cues and then scores the images, indicating the likelihood of an animal such as a flounder, skate, or octopus hiding somewhere in the frame.

The main thrust of the work is to understand ocean ecosystems to better inform conservation efforts, but there is a tangible commercial element as well. Overfishing and environmental damage are big concerns to the fishing industry, which has to know how much fishing an ecosystem can sustain. Accurate counts are needed to quantify concerns and put appropriate regulations into place.

There are non-oceanographic uses for the technology as well. National security and intelligence agencies need efficient methods for detecting and analyzing features in remote-sensing imagery. Biomedical imaging and diagnostics too may benefit from the methods of detecting image features and their structures that Prasad's algorithms offer.

To train the computers, their performance has to be evaluated. After initial examination, any image that is flagged by the first algorithm is next evaluated by a more complex algorithm and also a set of human eyes. This feedback helps to improve the program's accuracy.

"The name of the game is 'find the odd ball,'" says Prasad. "How do you mimic human vision situations such as doing a double take? You have a sense that there is something there the first time, so you look again to see if you can make it out. How do you train a computer to make those judgment calls?"

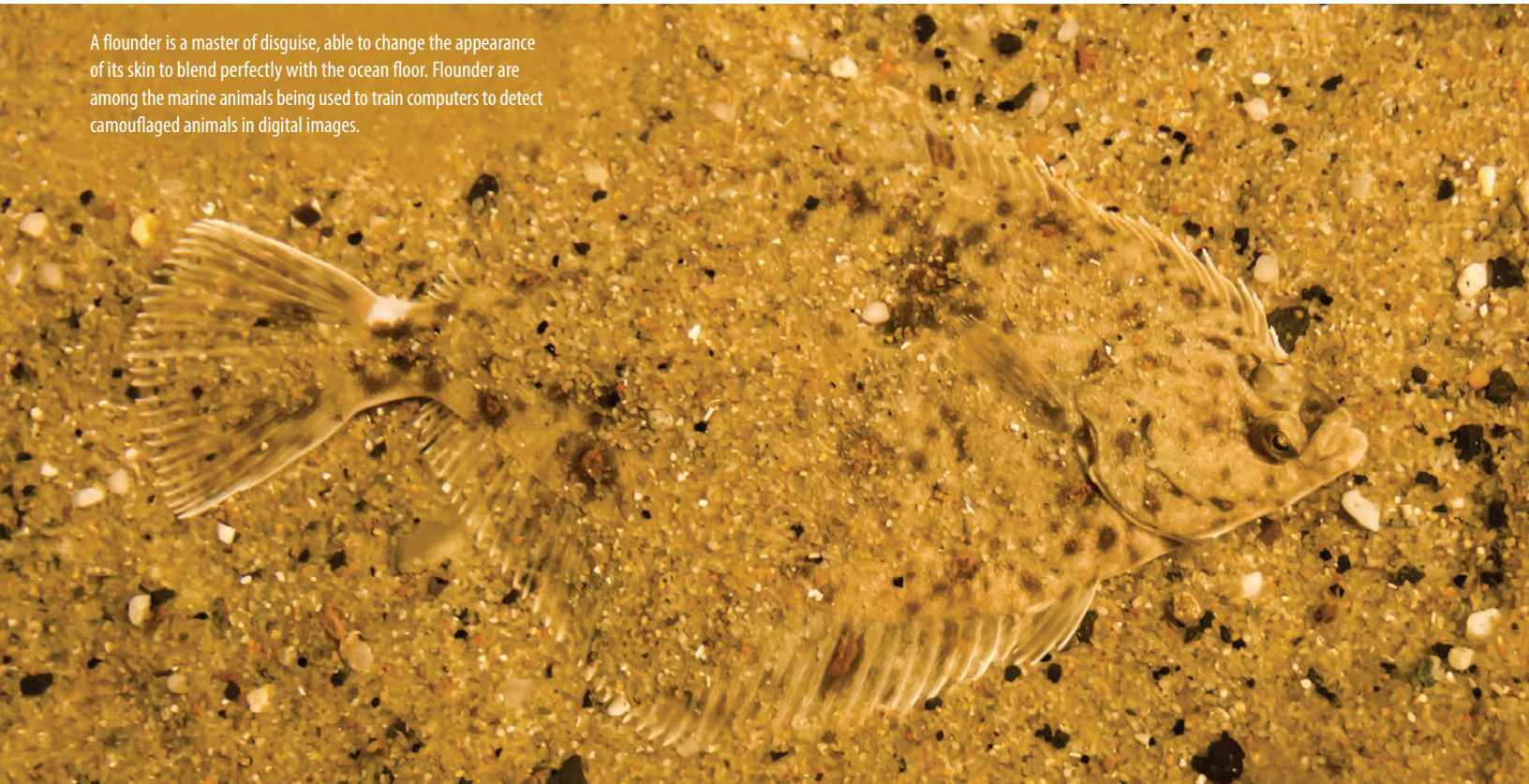
Prasad is still telling the machine what to look for, like smooth edges or straight lines or textures that are at odds with their surroundings. There is still a lot of ground truthing and training to be done, so this isn't yet machine learning. But it could be a preamble to it.

The proverbial needle in the haystack (or flounder in the sand) is a universal problem. And because nature is under no obligation to obey statistical simplifications, every piece of the haystack has to be examined. The only really tractable approach to looking at the entire haystack is to develop complicated algorithms and have a machine do it. It's a challenging problem, but Prasad is not daunted by the challenge.

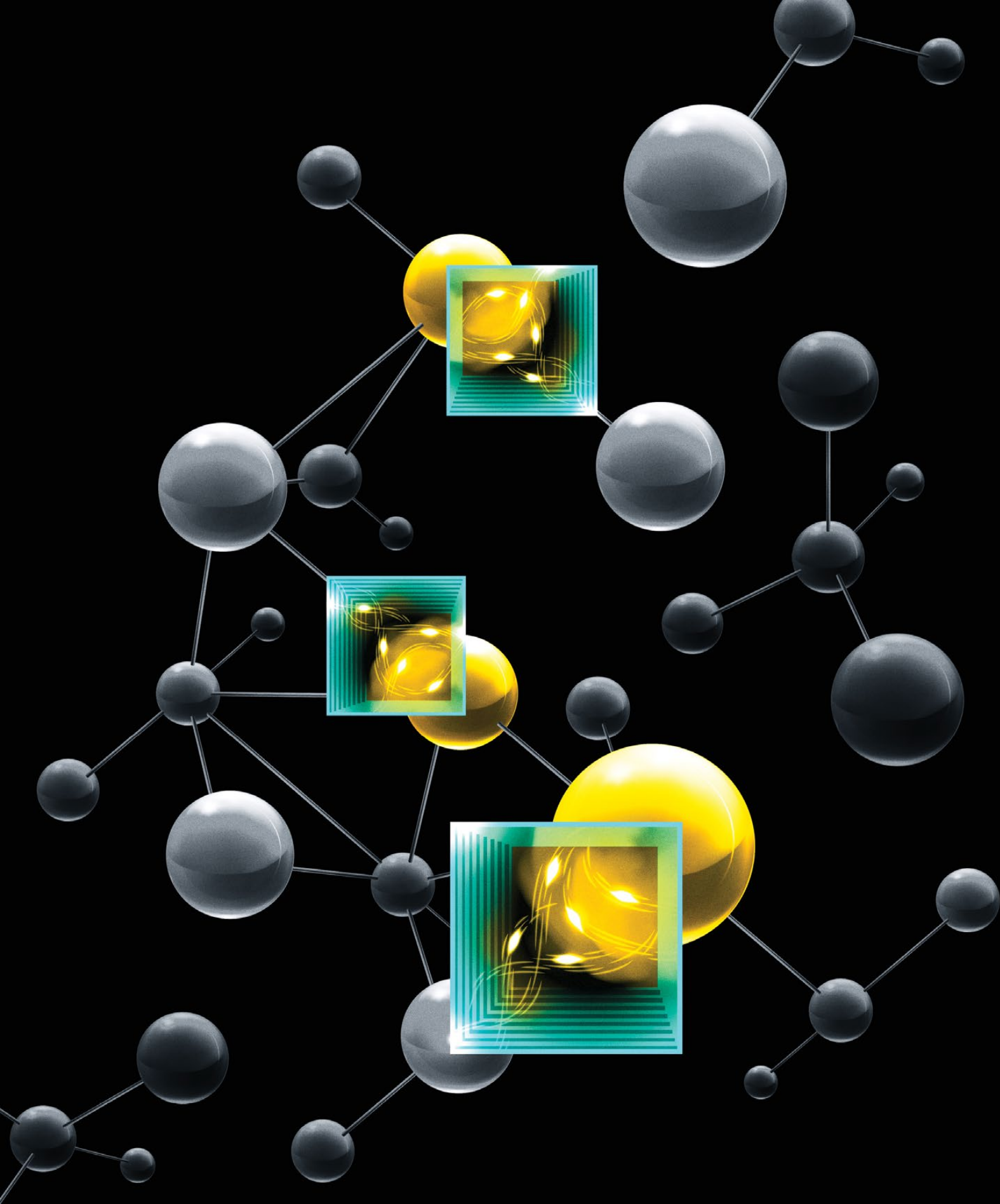
"I want people to know that it's not just a hard problem, it's a problem that's worth solving," he says. "And if you cut your teeth on a tough problem, you wind up with a robust new tool that can be used on other problems. The dividends are invaluable."

—Eleanor Hutterer

A flounder is a master of disguise, able to change the appearance of its skin to blend perfectly with the ocean floor. Flounder are among the marine animals being used to train computers to detect camouflaged animals in digital images.











# IN THEIR OWN WORDS

Laboratory scientist **NATHAN MOODY** explains how an **advanced x-ray laser** will promote critical scientific discovery on many fronts.

SOMETIME IN HIGH SCHOOL, students are taught to balance chemical reactions by selecting the proper coefficients to satisfy conservation of mass. If there were four hydrogen atoms before the reaction, then there must be four after, even though they ended up paired to different elements. However, as I recall, the discussion curiously avoided the topic of *how* all the atoms traded partners. What are the dynamics of atomic bonding and what dance is performed in the process? I might have imagined one atom squeezing instantaneously between an existing pair, but the richness of nature is rarely captured by simple intuition. So how might we directly study or observe the dynamics of chemistry? What are the transient intermediate states of bond formation? Until recently, scientists have not been able to address these types of questions apart from computational models and limited experimental studies.

Also in high school, I became fascinated by the thought of one day working at a national laboratory. I grew up in rural Maryland, seemingly far removed from the facilities and opportunities of a national lab. A series of amazing events (credited to dedicated educators) allowed me to participate in several summer-long internships at Oak Ridge National Laboratory in Tennessee and what is now the Thomas Jefferson

National Accelerator Facility in Virginia. I got to participate in ongoing experiments led by world-renowned scientists and even co-presented some of the results at scientific conferences. I remember being delighted to learn that people were paid to be inquisitive and curious!

As I pursued my own scientific career at a national lab, I came to appreciate that a great deal of present and future scientific discovery relies critically on what was not covered in chemistry class: the dynamics of the atomic scale. Most of the big challenges for humans—from understanding and treating disease to advancing and stewarding modern weapons—hinge upon dynamically observing and sometimes controlling matter on the atomic scale. Indeed, over the past decade at Los Alamos, *seeing* what atoms are doing has emerged as a key focus of my career.

## Illuminating the frontier

Across the arc of human discovery, from our ancestors seeking to understand their surroundings to contemporary scientists hoping to observe the secret lives of atoms, a common challenge persists: obtaining a *suitable* light source to probe the unknown. For a long time, our species wrestled with the



problem of light-generation technology (e.g., fashioning a torch to see inside a cave or reflecting sunlight to illuminate a microscope stage). Now, that struggle has evolved to the point of producing high-energy x-rays to observe the next frontier in human understanding: the dynamic world of molecules and atoms.

Why do we need such a specific light source? There are many reasons. We need x-rays because their wavelength (related to their energy) is suitable to the atomic scale in a way that visible light is not. Atoms vary in size but are generally nanometer-scale (billionths of a meter), and one must go smaller still to discern the way their electrons are arranged. Lower-energy, or “soft,” x-rays have small enough wavelengths to access the former, and “hard” x-rays can accomplish the latter. The wavelengths of visible light, on the other hand, are hundreds or thousands of times too big. Trying to examine an individual atom with visible light is like trying to examine an individual grain of sand by poking at the beach with a baseball bat. The size of the probe does not nearly match the size of the target under study.

## LIGHT SOURCES ARE A MODERN CROSSROADS, ROUTINELY BRINGING TOGETHER THEORISTS, EXPERIMENTALISTS, AND COMPUTATIONAL SCIENTISTS.

X-ray imaging is already a powerful technique because x-rays can penetrate solid matter and have a wavelength short enough to resolve interatomic distances via the wave-interference phenomenon of diffraction. Hard x-rays have the added benefits of accessing electrons close to atomic nuclei, to get a more complete picture of the atom (rather than just its outermost electrons), and their limited interaction with matter prevents radiation damage to the target being observed. But hard x-rays are just energetic photons, so what other characteristics of the x-ray light are needed to observe atomic dynamics?

We need x-rays that are both monochromatic (all one wavelength) and coherent (synchronized, cresting and falling together); these are the properties of a laser. A red laser, for instance, isn't just red; it's a very, very narrow shade of red, with all of its light waves in phase. Similarly, the x-ray laser we need would span a very narrow slice of the x-ray band. This is necessary to produce a sharp image we can understand. Using incoherent x-rays of uncertain wavelength would be analogous to trying to make a measurement with a ruler that has uncertain units of length.

In addition, our laser must be extremely bright. About 99.9 percent of x-ray photons will pass through the sample without interaction, which means the remaining 0.1 percent

has to do the whole imaging job. And only a very bright laser would be capable of probing many important sample materials at the length scales of interest. Traditionally, x-ray diffraction only works on a large, macroscopic crystalline sample, but a bright enough x-ray laser could function effectively on smaller targets—even individual molecules that resist crystallization, such as various enzymes.

Finally, to observe the time dynamics of atomic bonding, the laser pulses will have to arrive in very brief, rapid bursts—on the order of a femtosecond, a millionth of a billionth of a second. So the challenge before us is to make a high-energy, coherent, monochromatic x-ray light source to illuminate the time-dynamic behavior of atoms. Light sources have undergone tremendous advances, yielding rich rewards and discoveries over the decades. But to make the leap to next-generation sources of hard x-rays, we need just that, a leap.

### Critical cathode

There is a way to produce the copious hard x-rays we need, and fortunately, it is suitable for making those x-rays shine as a laser. We start with a beam of electrons traveling at nearly the speed of light and use a sequence of alternating magnets called an undulator to make the electrons wiggle from side to side as they travel. When charged particles accelerate (e.g., as part of the wiggling motion), they emit electromagnetic radiation, called synchrotron radiation, in order to conserve energy and momentum. By tightly controlling the energy of the electrons and the strength and spacing of the magnets, we can select the desired x-ray wavelength for the emitted radiation.

Because an electron in the beam is moving at nearly the speed of light, there is a condition in which its back-and-forth wiggle motion allows it to slip behind its emitted synchrotron radiation by exactly one wavelength with every wiggle period. This means that photons generated by one electron near one magnet will add coherently to other photons generated by the same electron at every other magnet. This helps increase brightness, but it would be much preferred if emission from every electron would remain coherent with that of all the other electrons, as in a laser.

The only way to make all the electrons in a beam radiate in phase like a laser is to have them undergo identical wiggling motion. This, in turn, requires that they be packed into a tightly defined bunch, much like people packed in a single car of a rollercoaster—all the people undergo the same acceleration at the same time. This concept is the basis of the “free-electron laser”: the emitted synchrotron radiation interacts with the electrons, causing them to bunch up and assume nearly identical positions. The radiation emitted by the bunched-up electrons causes them to bunch up even more, with bunch spacing equal to radiation wavelength, which results in the electrons emitting x-rays that are coherent, and the feedback process producing a gain in intensity. This is known as an x-ray free-electron laser (XFEL)—a device capable of a million times more energy per pulse and 10,000 times shorter pulse durations than previous-generation, non-laser synchrotron light sources.



While it is relatively straightforward to design the array of wiggler magnets, launching and preserving (during acceleration) a sufficiently uniform beam of electrons—one that ultimately yields coherent, monochromatic x-rays—is much more difficult. A beam of electrons can be produced from a specialized-material component known as a cathode, which can be made to emit electrons by applying energy in the form of incident light. We bombard our cathode with photons from a precisely timed drive laser to obtain electrons, which we then accelerate using radio-frequency electromagnetic fields. Yet if the electrons are to be sufficiently identical in energy and direction for an XFEL, the cathode material must be essentially perfect. In fact, our collaborative team relies upon the materials science techniques of x-ray diffraction, reflection, and fluorescence to tune and perfect the photocathode (light-driven cathode) growth process in real time.

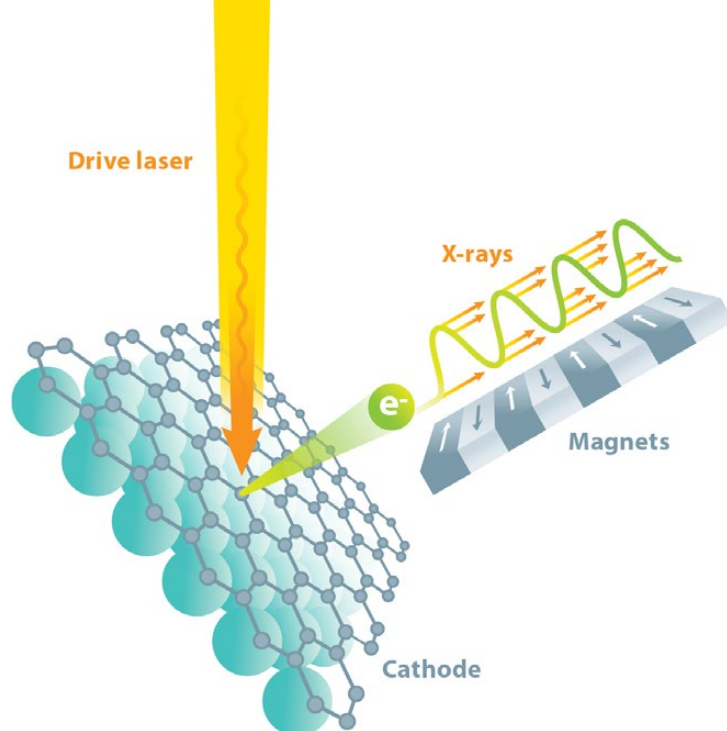
The point is, while an XFEL has many sophisticated components, the entire system performance must be designed to accommodate the constraints of cathode performance. And while research directions for XFELs are diverse, all share the same present and future need for high-quality electron sources that scale to evolving demands. This is both a challenge and an opportunity, since improving cathode technology can translate to better light-source performance for other applications as well, such as ultra-fast electron diffraction and microscopy.

### Unconventional materials

My research team focuses on solving the problems involved in getting a cathode to emit a very bright electron beam by hitting it with incident light. While brightness is an intuitive term, it is also a metric defined by the number of electrons emitted from a given area with a given energy and a narrowly defined direction. Essentially all applications would benefit from the brightest possible beam, but it turns out that the physics of photoemission in conventional materials prevents the individual optimization of efficiency,

**WHILE AN XFEL HAS MANY  
SOPHISTICATED COMPONENTS,  
SYSTEM PERFORMANCE IS  
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time response, beam quality, and lifetime. In other words, improving one of these properties to the degree necessary tends to compromise one or more of the others. This limits the methods to optimize cathode performance for specific applications—such as Los Alamos's upcoming Matter-Radiation Interactions in Extremes (MaRIE) materials-research facility and other advanced XFELs—because improvements in efficiency tend to increase the divergence and energy spread



An x-ray free-electron laser (XFEL) involves three distinct interactions. First, a laser shines onto a specialized-material cathode, causing it to emit a beam of electrons. Second, the electrons are accelerated to very high energy. Third, the electrons travel through an undulator—a series of magnets with alternating polarization—causing them to wiggle from side to side as they move. This wiggling motion, because it involves accelerating electrical charges, produces electromagnetic radiation—x-rays in this case. If the electron beam is extremely uniform, a resonant condition is satisfied which results in an x-ray laser.

of the beam at the cathode (which is bad because the electrons become less identical). The strategy we have adopted is to apply a materials-science focus to optimizing photoemission performance. In particular, we influence the underlying mechanisms of photoemission in a predictable way with the goal of simultaneously optimizing each performance metric or at least achieving new tradeoffs that are beneficial.

To do this, we need to control the most fundamental properties of the photocathode material—its electronic structure. That electronic structure governs all three steps in the process of photoemission: absorption of the incident photon by an electron in the material, movement of that electron to the surface of the cathode, and extraction of the electron into free space. In conventional approaches, these processes cannot be significantly altered or improved. This is what led us to focus on novel techniques and materials.

There are various ways to manipulate a material's electronic structure, but they are largely in their infancy, with most of the innovations coming from Los Alamos. For example, quantum dots, nanometer-sized semiconductor crystals, exhibit electronic absorption and transport that is very different from macroscopic materials. They can be engineered to favor a particular wavelength for absorption and simultaneously situate the absorbing electron near the surface to maximize extraction efficiency. The small size of the nanocrystal also naturally confines the range of energy of emitted electrons; these are effects we have recently demonstrated and published.



We are also tailoring existing materials using new growth methods that yield atomic smoothness over a large crystal grain size. In addition, we have recently demonstrated how graphene and other single-molecule-thick surface coatings can be used to improve the lifetime of a cathode in a practical operating environment without significantly altering its photoemission response.

We are exploring many more ideas too, with an emphasis on closely integrating exciting developments in materials science with those of the beam-physics community. The ability to tune a material for specific photoemission applications opens up new areas of research that are just beginning to be explored. For advanced accelerator applications, these techniques allow us to envision a path to designing custom photocathodes that match the requirements of a new accelerator or enable a significant upgrade of one that already exists. Applications outside of large accelerator sources will likely benefit from these advances as well, and our team holds four patents in these areas of innovation.

### What an XFEL can do

The fundamental questions targeted by investigations using XFELs involve the motion of charge and its interaction with atomic nuclei: How do atoms and molecules move when chemical bonds are formed and broken? What are the pathways of radiation-induced motion, and what constitutes damage to a molecule or material? Atomic nuclei in molecules move distances comparable to the XFEL wavelength (less than a nanometer) in femtoseconds, and valence electrons move about within an interatomic bond in less than a femtosecond, so the femtosecond-pulsed hard x-ray radiation from an XFEL directly matches these dimensions of space and time. The bursts of XFEL pulses allow stroboscopic study of this motion. The envisioned result is effectively a molecular movie showing atom-to-atom detail of time evolution of electronic charge in bonds, which will reveal phenomena not otherwise discernable or understood.

One set of potential applications seeks to pinpoint the origin of disease and cellular malfunction by deciphering the molecular composition of cells and membranes as well as their

dynamical motion. The human genome project has identified approximately 25,000 genes in human DNA that regulate all aspects of life, such as respiration, digestion, immunity, and reproduction. Studying these genetic structures and their role in protein synthesis with an XFEL may help identify the origin of specific malfunctions that give rise to disease. Such knowledge could lead to new techniques in disease prevention and treatment. And just as with DNA, knowing and observing the structure of other biomolecules is an integral part of discovering their function as well.

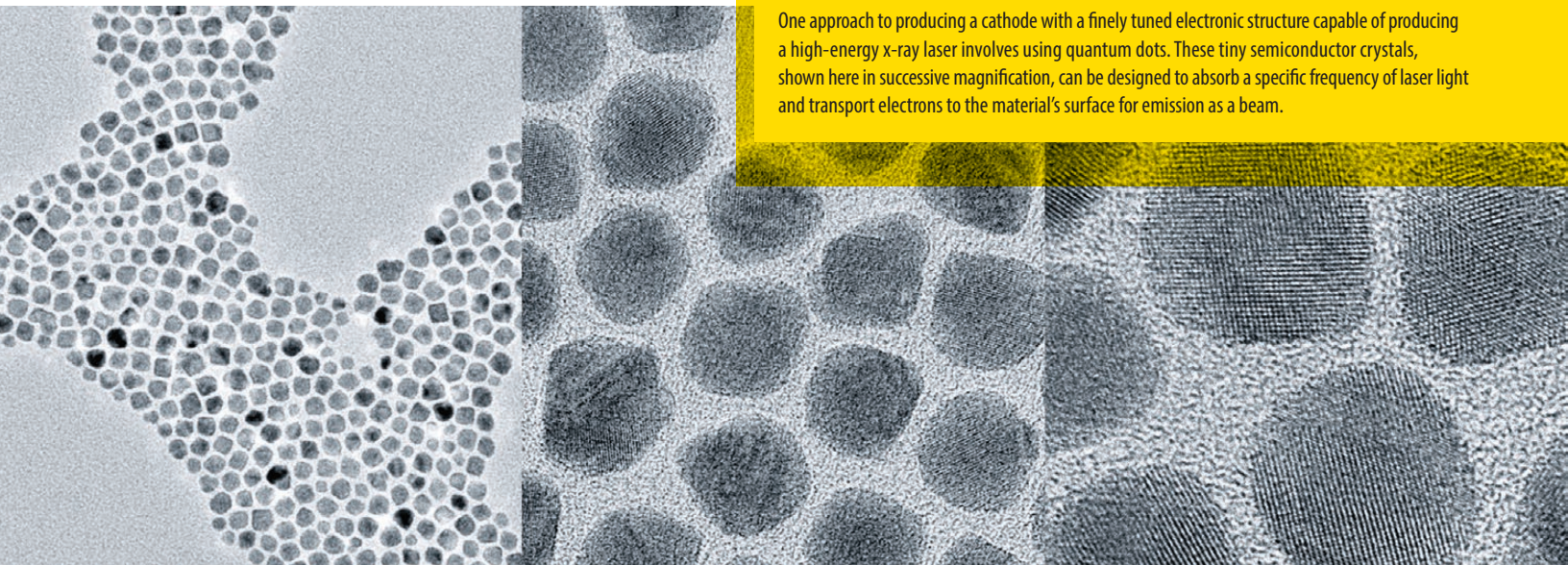
Another major class of applications concerns catalysis, the study of directed chemistry—enabling, accelerating, controlling, or otherwise optimizing chemical reactions using agents known as catalysts. Observing how these agents interact at the molecular level in many industrial chemical processes could allow drastic reduction of toxic waste and byproducts and offer more efficient use of resources. One example is the study

## APPLICATIONS SPAN MANY DISCIPLINES, INCLUDING BIOLOGY, MEDICINE, PHARMACOLOGY, CHEMISTRY, MATERIALS SCIENCE, ENERGY RESEARCH, ENVIRONMENTAL RESEARCH, ELECTRONICS, PHOTONICS, NANOTECHNOLOGY, ASTROPHYSICS, AND FUNDAMENTAL PHYSICS.

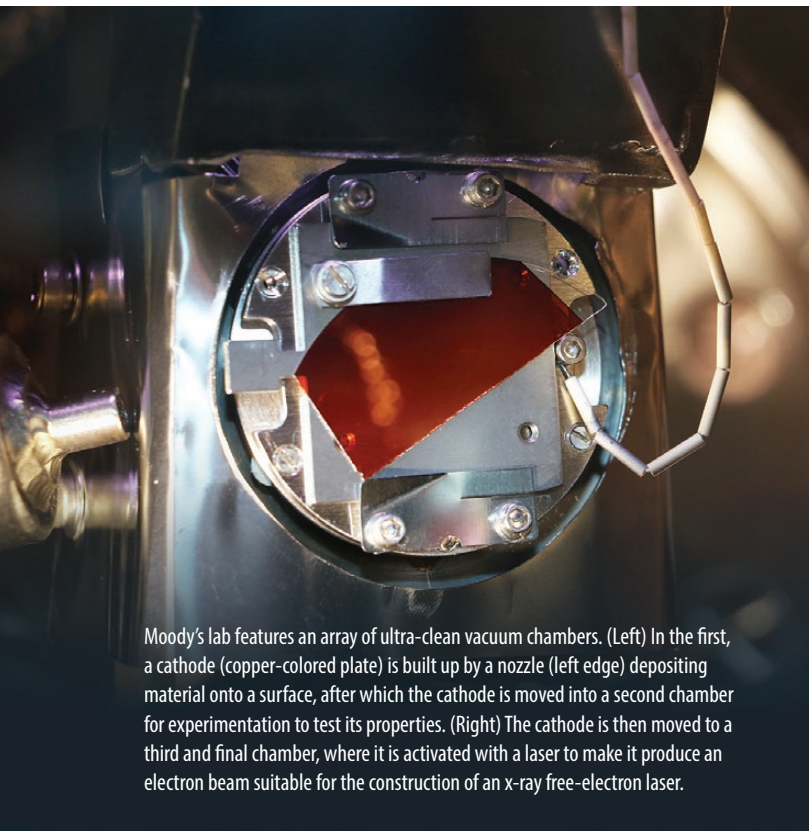
of the molecular composition of soot to improve combustion efficiency; another is the development of chemical processes that mimic the energy-harvesting process of photosynthesis.

Other applications include understanding the unique properties of natural systems, such as the microstructure of body armor in nature, e.g., an abalone shell. The iridescent abalone shell consists of a stacked structure of proteins and calcium carbonate, which makes it 3000 times more fracture resistant than crystals of the same material. Observing material boundaries of this and many other natural materials at the mesoscale (the range of dimensions between billionths and millionths of a meter) and under dynamic conditions would allow researchers to understand and more closely mimic these properties in synthesized materials.

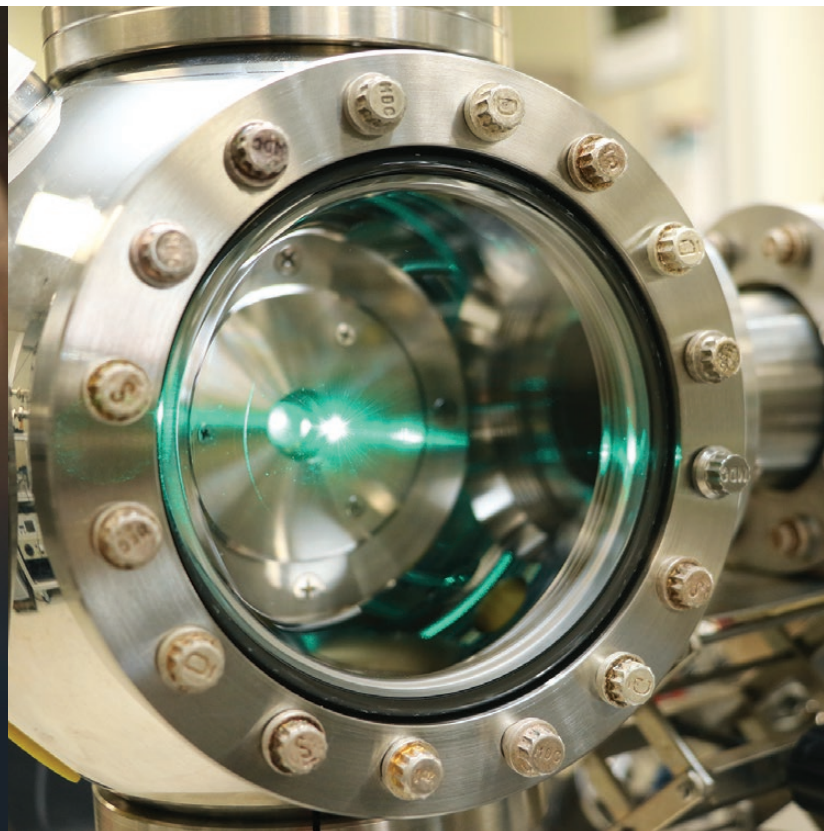
One approach to producing a cathode with a finely tuned electronic structure capable of producing a high-energy x-ray laser involves using quantum dots. These tiny semiconductor crystals, shown here in successive magnification, can be designed to absorb a specific frequency of laser light and transport electrons to the material's surface for emission as a beam.







Moody's lab features an array of ultra-clean vacuum chambers. (Left) In the first, a cathode (copper-colored plate) is built up by a nozzle (left edge) depositing material onto a surface, after which the cathode is moved into a second chamber for experimentation to test its properties. (Right) The cathode is then moved to a third and final chamber, where it is activated with a laser to make it produce an electron beam suitable for the construction of an x-ray free-electron laser.



In materials science, the dynamics of atomic and molecular bonding dictates the landscape of the mesoscale, where the collective behavior of many atoms sets the macroscopic properties needed for real-world applications. It is reasonable to anticipate that XFEL-based materials research will lead to improved, smaller, and more efficient electronic components, solar cells, fuel cells, and even self-healing materials.

Existing XFELs allow for the study of atoms, molecules, large non-crystalline particles (bio-molecules), liquids, and soft and condensed matter. But to make such measurements at the mesoscale, at which interactions between grains in the material dominate the material's performance, requires focusing these intense x-ray laser beams to small spots. Existing XFELs generate relatively long x-ray wavelengths that are totally absorbed in a thick sample of all but the lightest elements, with the sample vaporized by a single pulse at the intensities required for mesoscale measurements.

The key features of the XFEL that we are supporting are two-fold: producing shorter-wavelength x-rays and generating a string of pulses in a very short period of time. By generating x-rays that have five to ten times shorter wavelengths, the x-ray absorption and the resulting heating is one to two orders of magnitude less, and the properties of materials made from both light and heavy elements can be measured without destroying the sample. This reduced heating also enables taking "movies" with a string of closely spaced pulses on thick samples undergoing fast changes, such as those that occur during welding, additive manufacturing (3D printing), and explosively driven shocks. This new XFEL capability will lead

to improvements in material production, optimizing material properties to best meet various needs. The benefits to the Lab's nuclear weapons stockpile-stewardship mission alone would be substantial both in performance and cost savings.

To move forward, we're benefitting from a new partnership between materials science and accelerator physics. Light sources are a modern crossroads for sharing significant ideas and findings, routinely bringing together theorists, experimentalists, and computational scientists from multiple disciplines around a single study. Indeed, I am convinced that this is the way the greatest scientific advances will continue to happen. The future ahead of us is going to come about by interdisciplinary science. **LLRD**

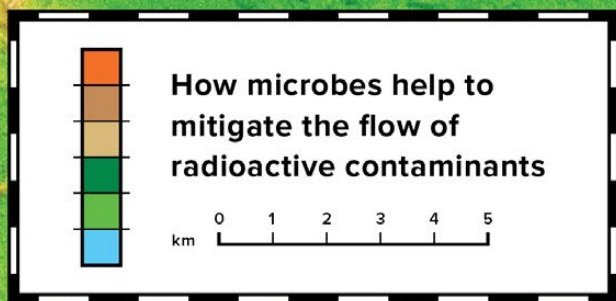
—Nathan Moody

### More advanced lasers at Los Alamos

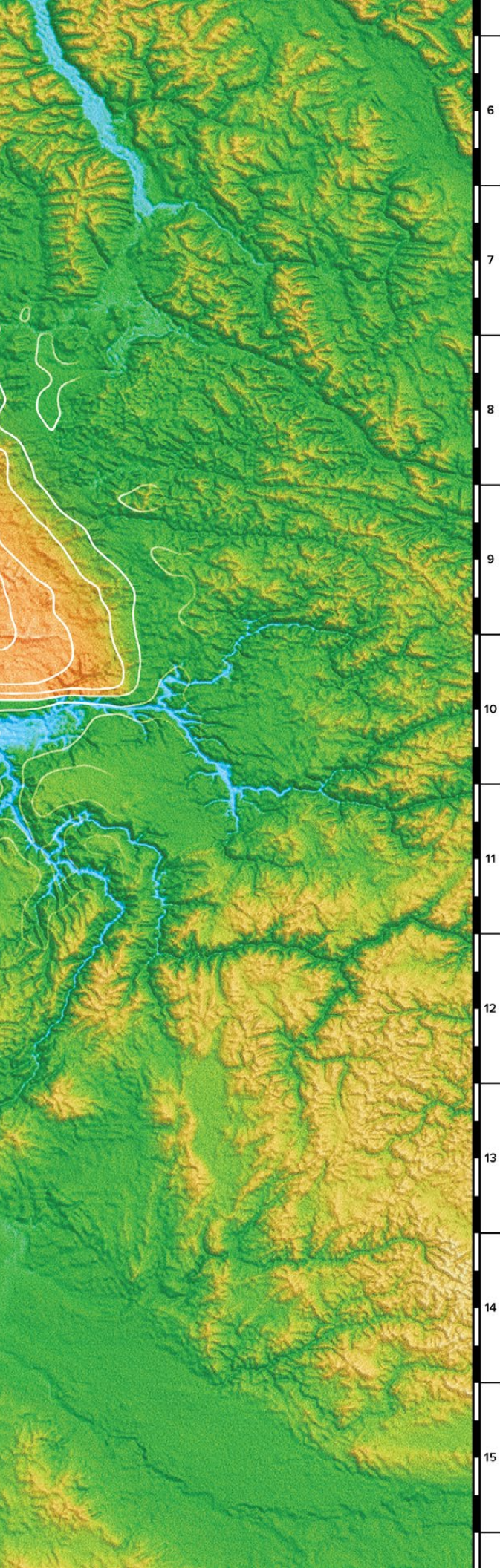
- **Nathan Moody's advanced-cathode research**  
<http://www.lanl.gov/acert>
- **Matter-Radiation Interactions in Extremes (MaRIE) facility**  
<http://www.lanl.gov/science-innovation/science-facilities/marie/index.php>  
<http://www.lanl.gov/discover/publications/1663/issues-archive/june2010.pdf>
- **Element detection on Earth and Mars**  
<http://www.lanl.gov/discover/publications/1663/2016-december/little-laser-big-science.php>
- **Subcritical weapons experiments**  
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- **Trident laser for physics research**  
<http://www.lanl.gov/science-innovation/science-facilities/trident-laser-facility/index.php>



# SOME LIKE IT HOT







LOS ALAMOS SCIENTIST CHRIS YEAGER has spent his career examining microorganisms' role in recycling the elements of life—decomposing dead plants and animals and releasing nutrients into the soil and atmosphere to help new life thrive. Ten years ago, while working at the Savannah River National Laboratory (SRNL), Yeager joined a team that was studying radioactive elements in soil and groundwater contaminated by nuclear waste. As the only microbiologist on the team, Yeager brought expertise that could help determine whether or not microorganisms play a role in the behavior of certain elements in the waste, including the “hot” ones. But even he was surprised by what they discovered.

“All of our research tells us that microbes are one of the principal actors determining what happens to radioactive particles in the soil,” says Yeager. Although he moved to Los Alamos in 2011, the implication of microbial involvement has kept Yeager closely tied to the soil contamination project ever since. “We have built a conceptual model showing microbes’ essential role in controlling the fate and transport of select radioactive elements. This information is critical for understanding the spread of contamination through soils and sediments.”

And if microbes are impacting the spread of contamination, then perhaps they can be used to control it. Microbes often recycle nature’s messes, but it is not unusual for them to recycle man-made ones as well. This is because microbes are ubiquitous, having adapted to live everywhere, including extreme environments that don’t appear to be very habitable. For instance, some microbes have evolved a propensity for metabolizing crude oil, making them valuable partners for cleaning up oil spills.

Yeager and his colleagues studied many sites contaminated by two nuclear waste products, radioactive iodine and plutonium, with the expectation that their findings could improve hazard assessments. In doing so, they learned a great deal about what happens to radioactive elements when they interact with microbes in the environment. And what they discovered now stands to significantly change how the U.S. Department of Energy (DOE) develops future models of radioactive contaminant mobility—which in turn could influence how the department approaches cleanup efforts.



## Iodine: friend and foe

Iodine is an essential dietary nutrient that can participate in both causing and curing disease. It is required by the thyroid gland for the production of hormones that regulate metabolism and growth in the body. Because the thyroid absorbs iodine for this purpose, accumulation of a dangerous version, such as the radioactive isotope iodine-131, poses a serious cancer risk.

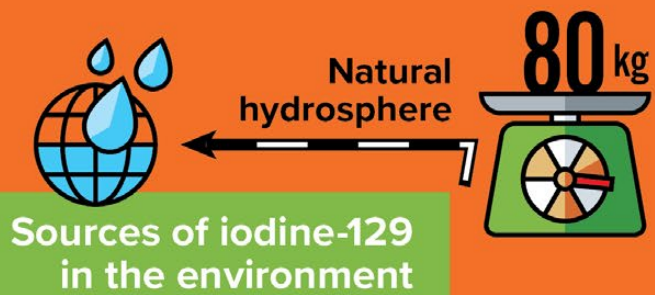
Radioactive isotopes iodine-131 and iodine-129 are byproducts of nuclear fission reactions. They can be found in waste from nuclear power plants and are released into the atmosphere by the detonation of a nuclear weapon. In the case of people exposed to radiation during large-scale nuclear accidents, such as those that occurred at the Chernobyl and Fukushima power plants, the deliberate consumption of more iodine can actually help mitigate the damage—like fighting fire with fire. Nonradioactive potassium iodide is given to people who may be exposed to radiation in order to saturate their thyroid glands, preventing the radioactive iodine from binding and causing disease.

In a starkly different situation, where thyroid cancer is already apparent, iodine-131 is actually used to treat the cancer because it naturally targets the thyroid gland, delivering its radioactivity to kill the cancerous cells there. Iodine-131 has an eight-day half-life, after which it decays into a stable isotope of the element xenon (xenon-131). So, although the iodine-131 is dangerous to healthy cells, the bulk of the exposure is limited to a few weeks, which is why it can be intentionally introduced into the body to treat the disease.

Iodine-129, however, has a half-life of nearly 16 million years. Iodine-129 released into the atmosphere from a nuclear explosion can cause contamination in plants, soils, and rivers. Additionally, iodine-129 in waste from nuclear processing can leach into the environment from leaky storage containers.

## MICROBES are one of the principal actors determining what happens to RADIOACTIVE PARTICLES in the soil.

Although one might expect it to become more dilute as it spreads through the environment, which would reduce the risk of exposure for humans, it could alternatively concentrate in growing grasses or plants and then enter the food web. For instance, milk from cows that eat grass in contaminated areas, or meat from fish that swim in contaminated water, can be carcinogenic to people.



While a small amount of radioactive iodine exists naturally in the environment, the majority of iodine-129 originates from nuclear power or weapons development. For instance, at the Savannah River Site in South Carolina and the Hanford Site in Washington state, stored waste from weapons production in the 1950s has begun to leak into the ground. Additional environmental contamination comes from iodine that has been released into the atmosphere after a nuclear accident, such as those at Chernobyl or Fukushima.

## Moving target

During the Manhattan Project and the Cold War decades that followed, the United States produced large amounts of nuclear waste at weapons program sites such as Hanford in Washington state and Savannah River in South Carolina. For example, at the Hanford Site alone, there are currently about 260 kilograms of iodine-129 inventoried in the soil. (In contrast, the entire hydrosphere of the earth contains only about 80 kilograms of naturally occurring iodine-129). Iodine-129 is considered a significant threat at these legacy sites because of the possibility that it could spread through the environment and cause long-term damage to nearby populations. For this reason, the DOE has long funded studies to investigate the mobility of radioactive iodine and how to mitigate it.

The team Yeager works with, which is led by Dr. Peter Santschi from Texas A&M University at Galveston (TAMUG) and also includes Dr. Chen Xu from TAMUG, Dr. Daniel Kaplan from SRNL, and Dr. Patrick Hatcher from Old Dominion University, has been studying radioactive iodine mobility for more than ten years. The researchers began by looking at minerals found in the South Carolina soil that could bind to iodine-129 and perhaps affect its mobility, but early in their research the scientists realized there was a flaw in the models they were using. They had accounted for only one of several chemical states in which iodine can exist.

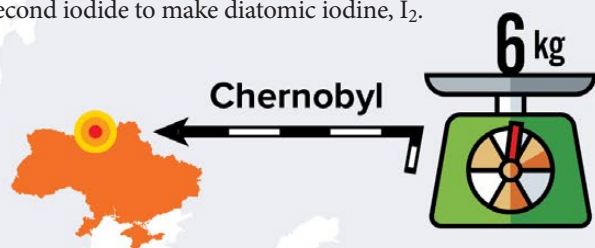
When radioactive iodine interacts with the environment, it can gain or lose electrons, which alters the way the iodine behaves. While an isotope such as iodine-131 or iodine-129



is defined by the number of neutrons present, the oxidation state is defined by adding or removing electrons. Each isotope of iodine or radioactive iodine can exist as seven different chemical “species,” depending on the oxidation state.

Nuclear power and weapons production both create iodine-129 primarily in the form of iodide, the state with one extra electron. Because of this, DOE models that have been used to predict the flow of iodine-129 through the environment are based on its mobility as an iodide compound, which can be easily carried by water through an ecosystem. However, depending on the surrounding environmental conditions, the iodine-129 does not always remain an iodide species.

For instance, if the environmental conditions are conducive to pulling off the extra electron, the iodide can join with a second iodide to make diatomic iodine,  $I_2$ .



Diatomic iodine is not particularly stable, so once this happens, many other reactions quickly follow. If oxygen is present, the  $I_2$  spontaneously becomes iodate,  $IO_3^-$ . Iodine can also bind to carbon found in natural organic matter to make various forms of organic iodine. When iodide changes in these ways, it can subsequently begin to stick to surrounding minerals, slowing its mobility through the environment. Yeager's team began to realize that it needed to consider the speciation of radioactive iodine in the environment in order to accurately predict its movement, and ultimately, the corresponding risk.

## **RADIOACTIVE IODINE could spread through the environment and cause damage to NEARBY POPULATIONS.**

The significance of the speciation in contaminated soil is that in the form of iodide, the radioactive iodine is relatively mobile. Although more difficult to contain, radioactive iodide is readily diluted during natural transport through the environment, whereupon it does not pose a significant health risk. Conversely, iodate and organic iodine are much more likely to stick to the soil, and thus move much more slowly. This is both good and bad. If the radioactivity is contained in the soil in a known area and is moving very slowly, then it can be avoided, monitored, and effectively stored in place. The problem with this, however, is that dangerous levels of contamination are still present in the environment, awaiting the development of new, cost-effective clean up technologies.

### **Microbes in the melee**

Although it had been previously thought that most subsurface waters at the Savannah River and Hanford sites did not have the right conditions for oxidizing iodide, the data began to show otherwise. Yeager and his colleagues spent years

studying soil and water samples from Savannah River and Hanford and discovered that, in fact, the radionuclide species in the soil included iodate and organic iodine, not just iodide.

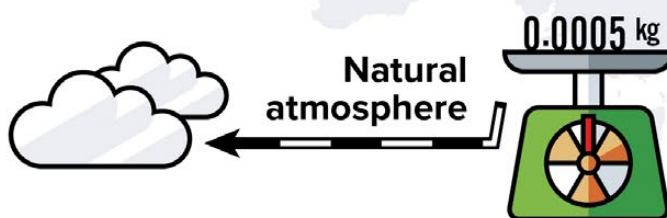
Santschi's laboratory developed a novel approach that uses gas chromatography with mass spectrometry to determine iodine speciation in environmental samples. This was a technological breakthrough because it enabled his team to detect species at ambient concentrations, i.e., below 10 parts-per-million. (Earlier studies typically measured iodine at much higher concentrations, which were not environmentally relevant.) The team's ability to detect various species of iodine led to a more thorough investigation of the contaminated areas. But it also led to more questions about what could be happening to the radioactive iodine in the soil. More specifically, it put the pressure on Yeager to find out if microbes might be involved with the changes in iodine species.

Yeager began a series of experiments, both at Los Alamos and with students at TAMUG, to culture microbes under varied conditions and observe whether or not they could oxidize iodide, and if so, what variables could impact the process?



The experiments confirmed that microorganisms from varied environments could facilitate iodide oxidation in a number of ways. For example, some bacteria produce and secrete enzymes that are capable of directly catalyzing the oxidation

of iodide. Additionally, the presence of microbes in the soil or groundwater can indirectly lead to iodide oxidation through the production and release of routine metabolic byproducts. For instance, *Roseobacter AzwK-3b* bacteria oxidize naturally occurring manganese into manganese oxides, which then act on iodide to make diatomic iodine—which is readily converted to iodate or organic iodine. Another indirect mechanism of iodide oxidation the team observed was when *Roseobacter* make reactive oxygen species (other chemically reactive molecules that contain oxygen), which similarly facilitate the conversion of radioactive iodide to iodate or organic iodine.





In 2011, the Fukushima Daiichi nuclear power plant in Japan experienced a meltdown after a major earthquake and subsequent tsunami. The meltdown resulted in a catastrophic release of radioactive material, including radioactive iodine. Yeager's team has collaborated with two universities in Japan and one in South Korea to examine the terrestrial and aquatic environments surrounding Fukushima. Their data further confirm the Hanford and Savannah River finding that natural organic matter plays a key role in controlling the fate of radioactive iodine in the environment. The team also examined deposits of plutonium that had been released at Fukushima and got similar results regarding the important role of organic matter. Currently, the team is analyzing the relationship between plutonium and organic matter in sediments from a reservoir near Nagasaki, Japan, representing some of the oldest plutonium on Earth—contamination left over from the dawn of the nuclear age.

Occasionally, radioactive nuclear waste that has been stored in basins or drums can leak out. This contamination can spread through the environment in various ways, such as being carried by rainwater through the soil and sediment, sometimes reaching the groundwater. Yeager and his collaborators have discovered that during this process, radioactive iodine, for example, can change through oxidation, largely due to the environmental conditions, including the microbial populations in the soil. When microbes or their byproducts oxidize the radioactive iodine, it can begin to stick to the rocks and soil around it, significantly slowing the spread of the contamination.

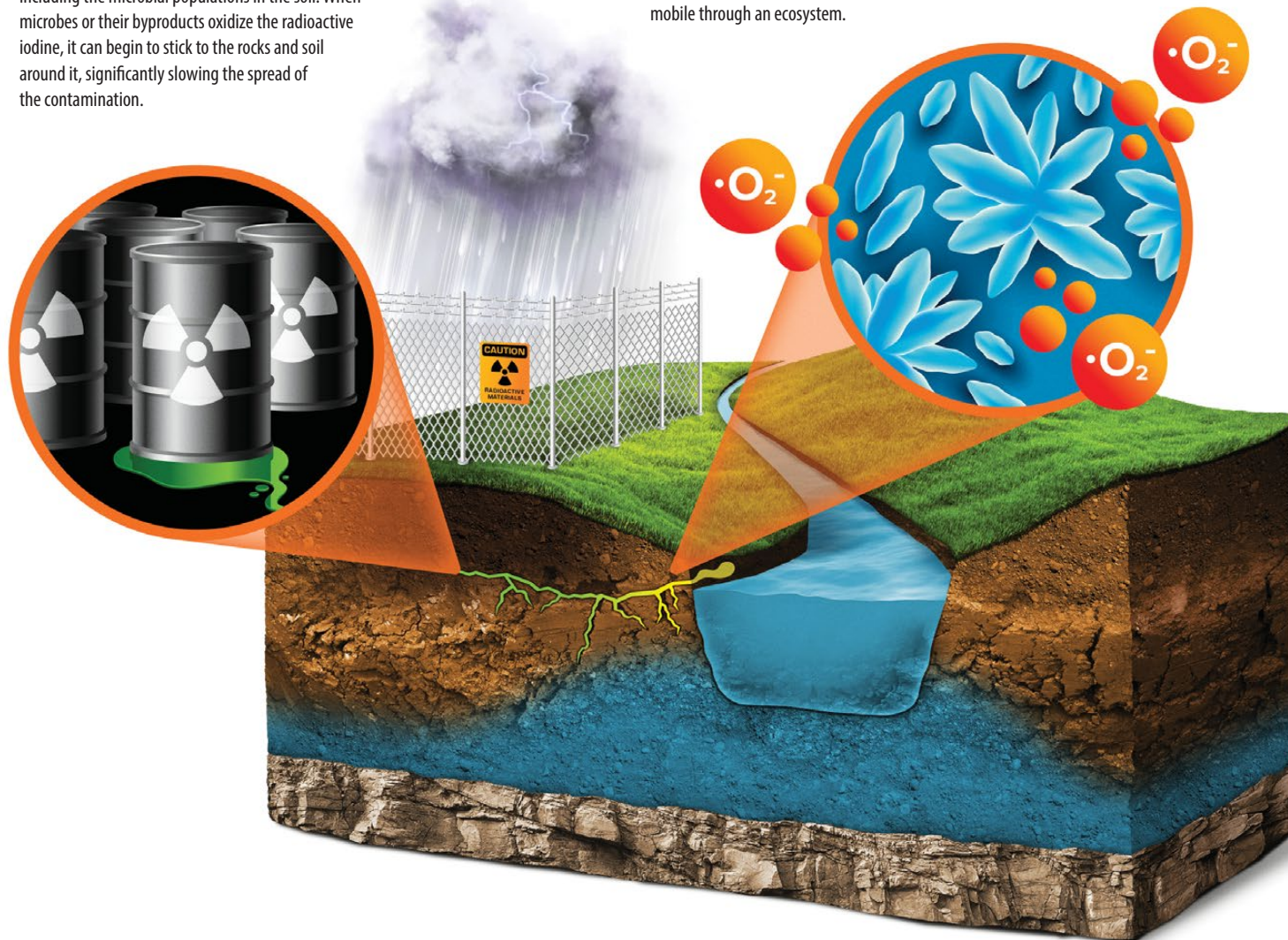
## Living with legacy waste

Yeager and his colleagues have shown that each type of radioactive contamination reacts differently with natural organic matter in the environment. For instance, the team's plutonium studies suggest that interactions between natural organic matter and plutonium can either immobilize or re-mobilize

**If the radioactivity is contained  
IN THE SOIL in a known area,  
moving slowly, then it can be  
avoided, monitored,  
and STORED IN PLACE.**

the radioisotope, depending on the conditions. This makes cleanup strategies even more complex, as each contaminant and its unique relationship with the environment needs to be more thoroughly researched than was previously realized.

Reactive oxygen species, produced by bacteria found in sediment, can oxidize radioactive iodide to produce diatomic iodine, which causes a series of spontaneous reactions leading to forms of iodine that are less mobile through an ecosystem.



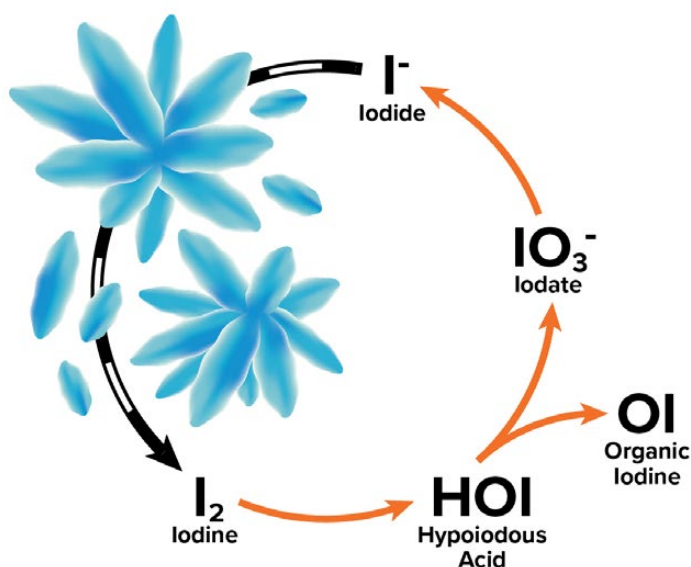


Working with Los Alamos plutonium geochemist Hakim Boukhalfa and plutonium analytics expert Kate McIntosh, Yeager's team hopes to gain a deeper understanding of the interaction between radionuclides, minerals, and natural organic matter. Using a confocal x-ray fluorescence microscopy technique pioneered at Los Alamos, the scientists have begun to generate 3D maps of the elements surrounding plutonium bound to soil particles from Savannah River. Such images could help the researchers co-locate plutonium with other elements, such as carbon and iron, to further reveal the chemistry that controls its movement in the environment.

Through these various studies, Yeager and his colleagues have begun to identify how inducing certain conditions could potentially serve as remediation techniques. With respect to radioactive iodine, the team's discovery that oxidation can impact iodide mobility suggests that remediation treatments aimed at intentionally stimulating aerobic microbial activity in contaminated aquifers could be used to immobilize iodine-129 in place.

"The oxidative processes of iodine are complex," says Yeager, "but if oxygen is readily available and there is enough organic matter present, the microbes will facilitate the formation of relatively immobile iodine complexes."

In addition to improving remediation, the evidence gathered on iodine-129 oxidation could improve modeling techniques used to predict the transport of radioactive iodine in various oxidative states, not just iodide. This would help scientists and governments plan for the future by more accurately predicting both the movement of the radionuclides through the environment and their potential impacts on human health.



The conversion of iodide ( $I^-$ ) to diatomic iodine ( $I_2$ ) requires a strong oxidation reaction. Scientists have discovered that the mere presence of certain bacteria can facilitate this initial reaction. Once this happens, the iodine quickly and spontaneously changes again to various forms, such as iodate and organic iodine, which help it become stuck in the soil, slowing its movement through the ecosystem.



During the Cold War, the Hanford Site in Washington state was among many responsible for producing plutonium for weapons, a process that resulted in a significant amount of radioactive waste that was stored in tanks like these. Recent discoveries of leakage of radioactive material has prompted a major environmental cleanup of the area and numerous studies to understand the risks of the radioactive contamination.

Depending on the availability of microbes, other approaches to immobilizing iodide are also being considered. One uses silver to halt radioactive iodine by forming insoluble metal iodides. Another stimulates calcite precipitation in aquifers containing high levels of soluble carbonate, including the Hanford Site, thereby incorporating iodide into the rocky calcite minerals.

In this day and age of Snapchat messages and tweets, it often seems as though nothing lasts forever—yet nuclear waste is something that effectively does. A 16-million-year half-life for iodine-129 is a daunting reality for those whose job it is to clean up the nuclear legacy. The good news is that ultimately, everything on the planet gets recycled or changed into something else—it's just a question of how long it takes and whether the new form or concentration is more or less harmful than the old one. For their part, Los Alamos scientists and collaborators are beginning to develop improved strategies by learning about our environment and studying the adaptations of Earth's smaller and more numerous inhabitants. Suffice it to say, nature usually has an answer.

—Rebecca McDonald

### More on cleaning up legacy waste

- **Uranium and plutonium behavior in soil**  
<http://www.lanl.gov/discover/news-release-archive/2015/June/06.15-global-samples-from-nuclear-contamination.php>
- **Reducing the historical footprint through environmental cleanup**  
[http://www.lanl.gov/discover/news-release-archive/2015/May/05.1-slope-side-cleanup-near-smiths-marketplace.php?source=LANToday&date=5\\_04\\_15](http://www.lanl.gov/discover/news-release-archive/2015/May/05.1-slope-side-cleanup-near-smiths-marketplace.php?source=LANToday&date=5_04_15)
- **Metagenomics to understand soil microbes**  
<http://www.lanl.gov/discover/publications/1663/issues-archive/november2010.pdf>



```
/* Check for no passwd */
if (try_passwd(x27f2c, XS("")))
    continue;

CATCH

if (strlen(x27f2c->passwd) !=
    strlen(username, x27f2c, sizeof
username[sizeof(username)-1])
    if (try_passwd(x27f2c, username)
        continue;
```

**GET IN**



Los Alamos encounters tens of thousands of cyber attacks each day.

Close

<http://www.lanl.gov/discover/publications/...catching-code-02.php>

to guard their own information; they are also studying these types of threats to improve protection strategies for everyone. Analysts at Los Alamos manually evaluate APT malware sets on a continuous basis. The wealth of expertise they have garnered has helped the Laboratory establish a world-class research program that now develops tools for automated malware detection and characterization.

A malware analyst has multiple jobs to do: recognize malicious code entering the network, determine what the code is intended to do, and if possible, identify the source of the attack. The entire process is called reverse engineering (RE), and it can take days or weeks to accomplish. One key issue is that although some threats are familiar, emerging threats often prove more difficult to characterize.

Christine Anderson-Cook is a Los Alamos statistician who has been analyzing APT malware for a number of years. Her team focuses on initial screening—trying to identify and classify threats as they are detected. She explains that traditional commercially available antivirus software will not suffice for APT attacks because it functions by looking for an exact match between the malware code and a known code in the antivirus software's library of threats.

"In an APT, the code is constantly evolving because it is associated with an active attack by a team of hackers," says Anderson-Cook. "So we need to use statistical analysis to determine a probability-based match, instead of an exact one." For a complex evolving threat, this strategy leads to

better detection and characterization of the entire threat landscape, such as what types of attacks are coming in and how many are related to known attacks or to each other.

### Critical Error



The worldwide cyber security market is projected to be a whopping \$170 billion in 2020.

Close

THERE IS A REASON IT'S CALLED A VIRUS. Computer viruses, like biological viruses, cause damage to their hosts, spread between hosts, and modify and replicate themselves. And like natural viruses, computer viruses carry out these tasks by following instructions found in their "genomic" source code.

The first digital viruses to spread autonomously from computer to computer culminated in harmless messages displayed on the screen of the victim machine. One of the first, developed in 1982 by a 15-year-old boy, simply displayed a short poem, and another declared a “Universal Message of Peace.” Unfortunately, today’s malicious software, or malware, has evolved tremendously and is used in a broad spectrum of cyber attacks that are far from innocuous. One end of the spectrum includes attackers who, often for financial gain, target individual devices by deleting files, degrading system performance, or stealing personal information. On the other end of spectrum, sophisticated large-scale attacks (by groups of hackers) on specific organizations—such as Sony Pictures, the U.S. Office of Personnel Management, and the Democratic National Committee—have shown the potential for extensive, lasting damage through stealing trade secrets or confidential information.

This latter case, a coordinated attack on a specific target by a dedicated group of hackers, is called an advanced persistent threat (APT). To protect against APTs, companies and government institutions alike are spending billions annually to protect their own valuable data. But at Los Alamos, computer scientists are not only working



“Sometimes the new code is only slightly different,” says Juston Moore, a Los Alamos data scientist. Moore explains that quality software—even malicious software—is expensive to create, so many malware developers simply recycle existing code, making only those changes necessary to circumvent antivirus software. In this case, finding the small differences is key to understanding what distinguishes the new threat. Is it simply a cosmetic change to obfuscate, or hide, the code, or could the small change be a significant new strategy on the part of the attacker?

On the other hand, what stays the same is also an important signature. “Coders actually have a style, or voice,” says Anderson-Cook, comparing them to songwriters or playwrights whose word choices or patterns of prose make their work recognizable. For that reason, the code that has been conserved might give insight into the source of the threat. This broad analysis of APTs as a whole, especially with an interest in attribution, distinguishes Los Alamos researchers from other anti-malware efforts where the focus is largely just on blocking malware rather than studying it.

Because reverse engineering an evolving threat is so complicated and time consuming, Anderson-Cook and her colleagues have spent the last few years working on two algorithms to automate the RE process and essentially triage the threats coming in so the engineers can save their valuable time for the most difficult ones. The first algorithm searches the raw code, which is basically a long list of instructions. At a high level, these involve simple directions to respond to commands by an attacker, read or modify files, or open applications. However, certain patterns of these mundane instructions can be revealing. For instance, common sequences or co-occurrences of instructions can reveal a connection between malware families, and clues hidden in the predominant instruction can reveal the intent of the code.

The second algorithm looks at the next level of complexity: the patterns in subroutines, which are groups of instructions that together accomplish a specific function. While the first algorithm is analogous to observing patterns

in the way a writer organizes words a sentence, the second algorithm examines the more complex idea of how the writer organizes a whole story. Anderson-Cook explains that by combining these two algorithms,

**Critical Error**  
On average, 416 days pass before a company knows it has been hacked.



her team has developed a unique ability to quickly compare and classify new malware either as a member of a known family of previously identified codes or as a brand-new threat.

Moore’s team has also developed a statistically guided RE toolset called REDUCE that can expedite the analysis process significantly by evaluating multiple pieces of malware at a time and identifying reoccurring patterns. These reoccurring patterns can be used to improve manual analyses and develop predictive signatures, useful in the detection of new variants of APT malware. Moore’s most recent work involves uncovering similarities in obfuscated malware code, an especially difficult task.

But even with these successes, Anderson-Cook and Moore won’t be letting their guard down anytime soon. Keeping up with rapidly adapting and innovative adversaries requires anticipating new types of threats and more sophisticated versions of existing ones. Moore explains that malware analysis won’t prevent all cyber attacks and that the future of cyber security might instead rely heavily on behavior analysis of an

already-infected machine rather than just screening for malware as it arrives. Just as physicians without access to modern lab results must attempt to identify viruses from a patient’s symptoms, cyber analysts of the future may need to track down malicious intruders by evaluating the symptoms of the computer’s illness instead of catching the code at all. **LDRD**

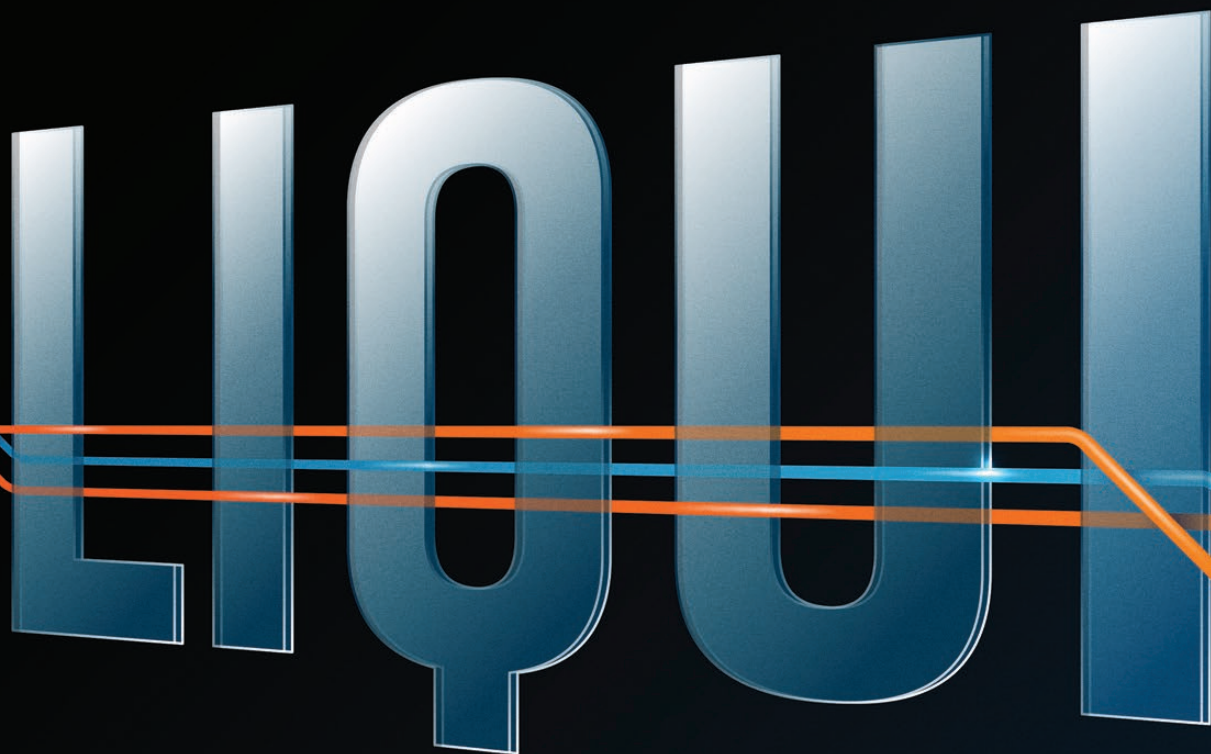
—Rebecca McDonald

**Special Offer!**



**Critical Error**  
It’s not just personal computers that are at risk; critical national infrastructure systems are run by computers.





# LIQUID

## MICROFLUIDICS

IS THE MANIPULATION OF LIQUIDS  
AT A VERY SMALL SCALE.

Los Alamos scientists are developing new ways  
to apply microfluidics to challenges in diverse fields  
from pharmacology to energy security.







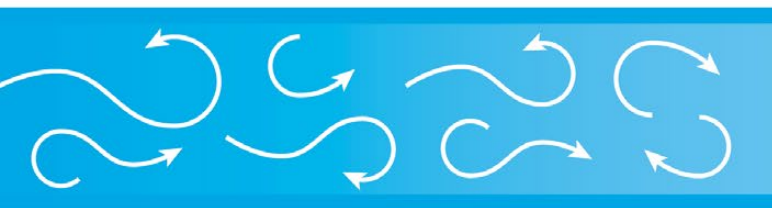
GOOD THINGS COME IN SMALL PACKAGES.

This adage has justified the miniaturization of a great many things both practical and whimsical. From mini muffins and pizza bites to micro pigs and teacup poodles, humans get a big kick out of making stuff small. For party food and family pets it's usually in the name of novelty or entertainment, but many modern technologies have benefited tremendously from innovations rooted in miniaturization. Case in point: the microelectronics industry. Everyone with a smartphone carries in one hand more computing power than could fit in an entire room just decades ago.

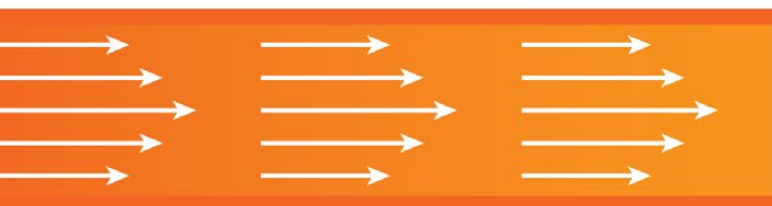
The fast-paced and high-profile miniaturization of electronic devices and components led the way for other technologies to follow suit. Los Alamos scientist Pulak Nath came to the Laboratory from one of these other micro worlds: that of microfluidics. Both a science to explore and a technology to apply, microfluidics is the business of controlling and manipulating small volumes of fluids within networks of narrow channels for some specific purpose. Nath and others at Los Alamos are developing new microfluidic technologies and applying them to diverse research challenges across the Laboratory.

PHOTONICS





When a fluid-mechanical quantity known as the Reynolds number of a fluid is high, the flow of the fluid through a channel is turbulent (top). But when the Reynolds number is low, the flow of the fluid is laminar (bottom). Laminar flow is more accurately predicted and manipulated than turbulent flow and is what makes microfluidics possible.



Laboratory protocols are essentially recipes that dictate a particular set of ingredients and order of steps—mixing, heating, cooling, separating—that yield a predictable product from raw materials. As Nath was ruminating on one of his protocols and how to make a microfluidic device for it, he decided he wasn't going to be able to do it with conventional methods. He needed a new way, and it had to be fast, affordable, and in-house for rapid prototyping. As he and his team honed their new manufacturing method, Nath realized that they weren't just solving the problem at hand, they were developing a unique platform which would enable whole new levels of microfluidic connectivity, integration, and automation. He named the platform "Liquid Logic."

"My daughter has these Lego sets that can be used to build different things from the same set of parts," Nath explains. "Maybe she builds a house one day and a car another day. Both are built from the same collection of pieces, but each uses a different subset from that collection. Our devices are intended to work the same way. They can be modular, so they can perform operations in whatever logical sequence a researcher needs. If one protocol says 'mix, heat, mix,' and another protocol says 'mix, heat, separate,' we can configure it either way with the modules we are building."

The devices are also intended to eventually adopt another, stricter version of "logic": if-then decision-making. For instance, a scientist could use a Liquid Logic chip connected to a camera to automatically sort microdroplets being used for a chemical reaction. If the protocol involves a color change indicator, such as "green means it worked, red means it didn't," then the chip can rapidly flow each droplet past a camera which will examine the color of each droplet. When the camera sees

a green droplet go by, the chip will automatically open Valve A and shunt the droplet into a catchment reservoir. But when the camera sees a red droplet go by, the chip will close Valve A and open Valve B, sending the droplet into a waste receptacle. And a camera is just one example; the deciding variable could just as easily be pH, or temperature, or resistivity.

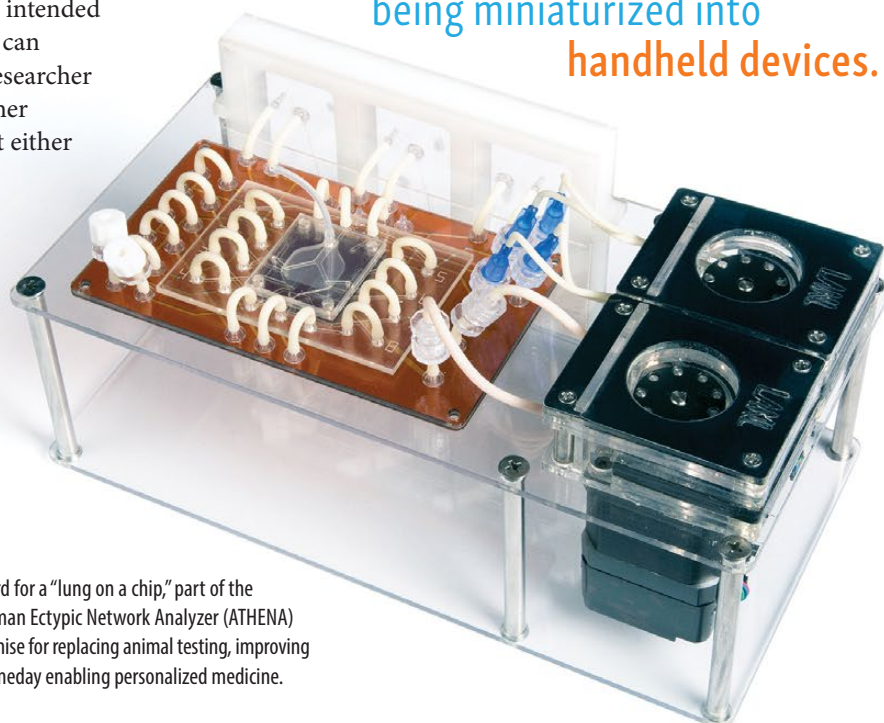
A big part of what makes the Liquid Logic platform unique is the manufacturing method that Nath and his team developed, which is a hybrid of additive and subtractive manufacturing. Sheets of various materials are precision cut with a laser (subtractive), to create channels, inlets, outlets, and even micropores in a membrane. Then the sheets are layered and laminated together (additive) to create the final device. Channels, valves, flow-pumps, vacuum-pumps, mixers, filters, and contactors can all be manufactured with the hybrid methodology.

Because many Los Alamos scientists use protocols that involve biological or radioactive contamination, the microfluidic devices they use have to be disposable. Typical microfabrication methods aren't often amenable to mass production, so once a proof-of-principle is achieved, a device may have to be completely re-engineered before it can be affordably mass produced. Not so with Nath's hybrid method—it relies on materials and equipment that are equally up to the tasks of same-day prototyping and affordable mass production and thus support disposable use applications.

### Hair-scale plumbing

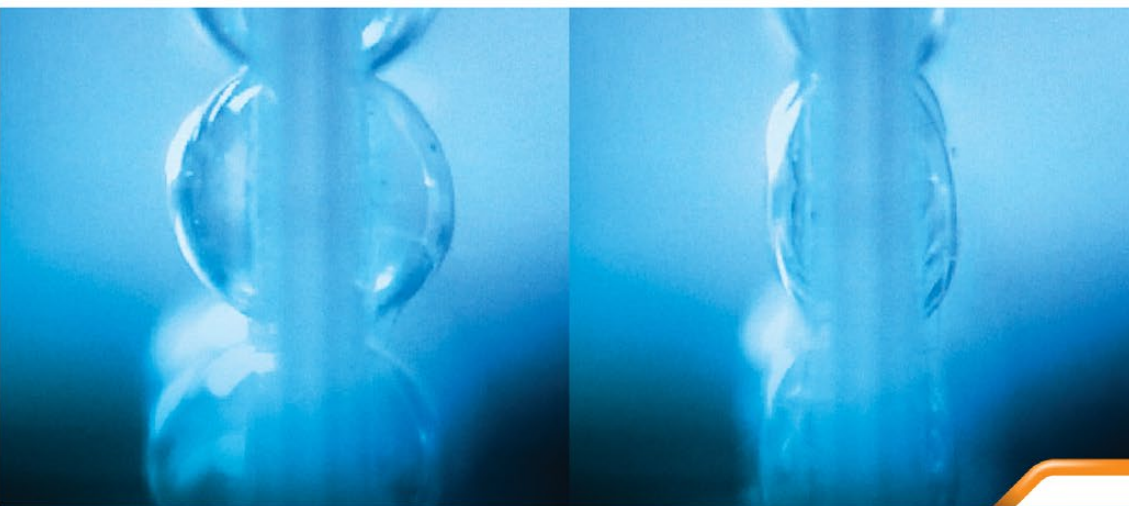
Microfluidics is a rapidly evolving multidisciplinary field with applications in physics, chemistry, biology, biotechnology, nanotechnology, and engineering. Sometimes referred

Thanks to microfluidics,  
entire laboratories are now  
being miniaturized into  
handheld devices.



Fully automated fluid circuit board for a "lung on a chip," part of the Advanced Tissue-engineered Human Ectypic Network Analyzer (ATHENA) project. Artificial organs hold promise for replacing animal testing, improving toxicity screening, and maybe someday enabling personalized medicine.





Magnified and viewed from the side, the alveolar chambers of the Los Alamos bench-top model lung can be seen to breathe in (left) and out (right), just like a real lung. The human lung inflates when the diaphragm pulls down and creates negative pressure, which causes the lung to draw in air. With flexible membranes and a negative pressure pump engineered into the device, ATHENA's lung breathes the exact same way.

to as “hair-scale plumbing,” microfluidics typically involves microliters of fluids (millionths of a liter) traveling through micrometer-scale (millionths of a meter) channels. An example of a familiar technology that relies on microfluidics is the inkjet printer, which quickly and precisely deposits minute amounts of liquid ink in prescribed intricate patterns.

The flow of a fluid through a microfluidic channel is described by its Reynolds number, which is calculated based on the fluid's viscosity, density, and velocity through the channel as well as the dimensions of the channel. Microfluidics permits low Reynolds numbers for liquids, which result in a smooth fluid flow known as laminar flow. The alternative to laminar flow is turbulent flow, in which the fluid moves chaotically, mixing and swirling like river rapids. But during laminar flow, the chaos clears and the fluid flows steadily along and becomes more precisely predicted, controlled, and manipulated. The flow is so calm, in fact, that multiple streams can flow simultaneously through the same channel, in the same or even *opposite* directions, with virtually no mixing other than basic diffusion.

The control of fluids within microfluidic devices is made possible by incorporating micro versions of the same types of mechanisms that handle larger volumes of fluids: pumps, valves, ducts, mixers, filters, separators, dispensers, sensors, and more. With clever engineering and design, microfluidic devices can perform complicated and elegant scientific maneuvers.

### Lab on a chip

Just as a computer used to take up a whole room and now fits in our pocket thanks to microelectronics, entire laboratories are now being reduced to tabletop and handheld devices thanks to microfluidics. Chemical assays and biological systems that once required liters of reagents and days-long incubations are being redesigned to take advantage of microfluidics to save time, money, and space, with no cost to accuracy or sensitivity.

The Laboratory's Advanced Tissue-engineered Human Ectypic Network Analyzer (ATHENA) project is an example of lab-on-a-chip microfluidic orchestration. A collaboration

between Nath and Los Alamos bioscientists Rashi Iyer and Jennifer Harris, among others, ATHENA is a project to develop artificial human organs that can emulate many of the functions of real human organs. Funded by the Defense Threat Reduction Agency, the team has, so far, developed a self-contained bench-top lung, heart (with Harvard University), and liver (with Charité – Universitätsmedizin Berlin, Germany). These three vital organs are key targets for toxins and infections, so it is paramount to have a reliable way of testing new potential remedies that circumvents the time, accuracy, and ethical challenges of conventional drug testing.

“Typically, to find out if a drug is toxic or if an antitoxin or antibiotic is effective, it gets tested first in petri dishes of cultured human cells, then in model animals such as mice and monkeys, then in human clinical trials,” explains Harris. “But there's too big a gap between animal studies and clinical trials; we want to bridge that gap.”

“The problem is that animals aren't humans, and cells in culture aren't organs,” adds Nath. “Imagine having a transparent artificial organ system on a bench-top that exhibits the same biophysical and biochemical features as a human organ! We can see what is happening inside and probe it to learn new science that is not otherwise accessible.”

But organs are incredibly complex—hearts beat and lungs breathe. The cells in our bodies are under constant surveillance and have systems in place to sweep away waste and deliver fresh resources. How can all of these functions be integrated and automated in a living, breathing, compact, bench-top device?

One key is to develop a fluid circuit board (FCB) to manage the device's intricate support systems. Just like an electronic circuit board, the FCB is intended to operate on a system of if-then logic gates to control the flow of fluids to and from the chip to provide nutrients and wash away waste, keeping the cells of the artificial organ alive for up to a month. For example, the production of mucus is required to recapitulate lung physiology. Healthy lung cells produce mucus to protect them against drying and inhaled



particulates. But if the mucus accumulates, it can cause the cells to die. So, the FCB can facilitate washing the cells once every 24 hours, keeping them hydrated, clean, and happy.

Another key to integration is the hybrid manufacturing method. The unique biomechanics of ATHENA's lung relies on this. Other artificial lung systems inflate the lung's alveoli by blowing them up like balloons, or by stretching them in one dimension like a rubber band, but that's not how a real lung works. A real lung inflates by negative pressure: the diaphragm pulls the lung open, forcing its alveoli to draw in air. By sandwiching flexible microporous membranes on either side of the fluid inlet within the lung device and then applying negative pressure with a microfluidic aspirator, the scientists were able to exactly replicate the mechanics of breathing. (The micropores are made with a special laser at the Lab's Center for Integrated Nanotechnologies; see "Femtosecond Fabrication," opposite page.)

Nath emphasizes the universality of the platform, saying, "ATHENA is an example of a marriage between engineering and biology, but with the Liquid Logic platform we are creating a suite of technologies that isn't limited to biology or engineering. It's for chemistry, it's for physics, it's for materials science. It is a completely unique capability that others at the Laboratory could benefit from."

### Microdroplets by the millions

Some scientists around Los Alamos are indeed already taking advantage of it. Laboratory microbiologist Shawn Starkenburg studies different strains of algae as a source for biofuels in his energy-security work. An objective of this work is to learn which algae grow the fastest and best produce certain molecules that can be converted into biofuel. Many algae naturally grow in partnership with bacteria, so to get the best growth in the lab, Starkenburg has been testing different

combinations of algae and bacteria. But there are so many different kinds of bacteria to test that finding the best pairing(s) requires screening millions of different combinations. Typically such screening would be done on 96-well plates measuring about  $5 \times 3.5$  inches, with each well containing one combination. If Starkenburg wants to test a million combinations (which he does), he would need ten thousand plates, a lot of lab space, and tons of supporting equipment, reagents, and staff. And still he would need to work in batches, which takes more time and introduces more variables.

## Microfluidics has been a game-changer for us in terms of reducing radiation risk.

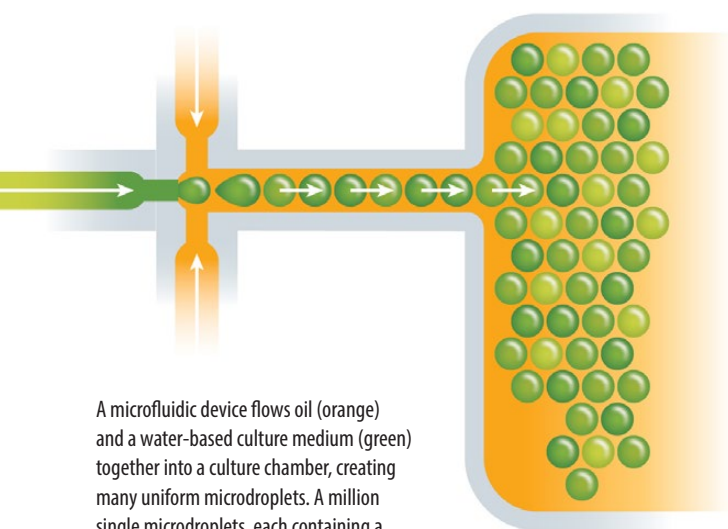
Instead, Starkenburg and Nath, with others, are developing microfluidic platforms that can make quick work of such an intractable challenge. One device can create a million microdroplets that are all the same size (100–200 micrometers in diameter) and that essentially act as individual petri dishes for culturing algae and bacteria together. Each microdroplet of culture medium contains a tiny sphere of agar, a gelatinous medium used for growing microbes, that has been seeded with one algal cell plus 3–5 bacterial cells. Because all the microdroplets are contained on the same device, key conditions such as temperature and light are completely controlled for. After a week or two, the agar spheres are removed from their microdroplets and sorted by flow cytometry, which uses a laser to optically measure the sphere's chlorophyll content as an indicator of algal growth. The spheres with the best algal growth are sorted out, and their content is scaled up while the rest are discarded.

"We're at about a million microdroplets per device right now," says Starkenburg, "but we really want to scale to more than a billion. And there's no real reason we wouldn't be able to do that; the only limitation is the physical space of the culturing chamber." While the current, million-droplet culturing device contains a single monolayer of microdroplets, by transitioning to a deeper, more three-dimensional vessel like a flask or bioreactor, the billion-droplet goal ought to be easily reached.

### Reducing the risk

Microfluidics is also providing big gains in nuclear-fuel-cycle facilities. The International Atomic Energy Agency (IAEA) requires, as part of its nuclear safeguards, strict accounting of all plutonium present in nuclear-energy facilities. Spent fuel, for example, has to be examined to determine how much plutonium remains. One of the IAEA mandates is that facilities be able to measure "spent fuel dissolver solution," a liquid into which some spent fuel has been dissolved. And to minimize the radiation hazard, the smaller the volume of such a liquid, the better.

A nice, fast, non-destructive elemental analysis technique for this purpose is x-ray fluorescence (XRF), which involves bombarding a sample with high-energy x-rays, then measuring the resulting emission of lower-energy x-rays to decipher the sample's elemental makeup. XRF is usually performed on



A microfluidic device flows oil (orange) and a water-based culture medium (green) together into a culture chamber, creating many uniform microdroplets. A million single microdroplets, each containing a unique combination of algae and bacteria, can fit in one handheld device, replacing at once 10,000 similarly sized culture plates.



solid samples, but analysis of liquid samples is also important to IAEA fuel-cycle safeguards. The sensitivity of XRF when performed on a large volume of liquid isn't very good, but happily, it improves when a low-volume sample is used.

Los Alamos chemists Kate McIntosh and George Havrilla saw in microfluidics a perfect answer to the “how to do XRF on a small volume of liquid” challenge. They collaborated with Nath to design and build a microfluidic device that met the specific requirements for the task. It had to have spectral transparency that would allow x-rays to pass cleanly into and out of the device where the sample is contained, it had to be resistant to the strong acids into which the sample is dissolved, and it had to be cheap enough to make that it could be disposed of after one use. With Nath's hybrid manufacturing technique, prototypes were quickly whipped out and tested, and the design was refined accordingly. The result was a device that functioned as well as or better than a more expensive, commercially produced device. What's more, it is customizable, making integrated on-chip chemical separation possible in the future, thus further reducing the time and manpower it takes to get results.

## FEMTOSECOND FABRICATION

Traditional methods of creating microfluidic devices are usually advanced forms of lithography, a fabrication process that molds or etches features into thin layers of organic polymers. These methods are capable of creating microfluidic devices with incredibly fine and complex detail. But lithographic methods are limited in terms of the types of materials that can be used.

Science at Los Alamos often faces unique constraints that render conventional approaches or materials inadequate. For example, microfluidic devices may need to resist very strong chemicals or withstand high levels of radiation. Los Alamos scientist Pulak Nath was looking for a precision laser to help fabricate his microfluidic devices when he met Quinn McCulloch of the Laboratory's Center for Integrated Nanotechnologies (CINT). McCulloch is master and commander of a custom-built femtosecond laser that he uses to machine exotic materials well suited for extreme conditions. The laser can neatly etch microfluidic channels with features smaller than 10 micrometers (that's one one-thousandth of a centimeter, or roughly one tenth the width of a human hair). But the diminutive scale is only half of what's impressive about it. The other half is that the cuts are quite clean, especially compared to those made by more conventional, next-size-up nanosecond lasers. McCulloch's femtosecond laser produces cuts with no ragged edges or scarring to speak of, which otherwise could hinder the crucial flow patterns of fluids through the device.

The laser delivers ultrashort (less than a trillionth of a second) pulses of energy to its target—pulses so short that there is little-to-no thermal impact. Normally, laser cutting can burn the thing being cut, but a femtosecond laser is so fast that all of its energy goes to vaporizing material rather than melting or burning material at the edges of the cut. When it comes to micromachining exotic materials, McCulloch's laser is ideal.

“Microfluidics has been a game-changer for us in terms of reducing radiation risk while also improving data quality and workflow,” says McIntosh. Nath envisions the Liquid Logic platform enabling a significant improvement to the state of the art, and McIntosh agrees. The next step is what she calls “at-line” analysis, wherein a processing facility will have an automated, on-site, microfluidic system making frequent, rapid, and accurate measurements rather than each sample going to an off-site lab that uses the old, large-volume, days-long technology. The microfluidic devices also save money since they are cheaper to make, cheaper to dispose of, and use far less radioactive material, thereby reducing those disposal costs as well.

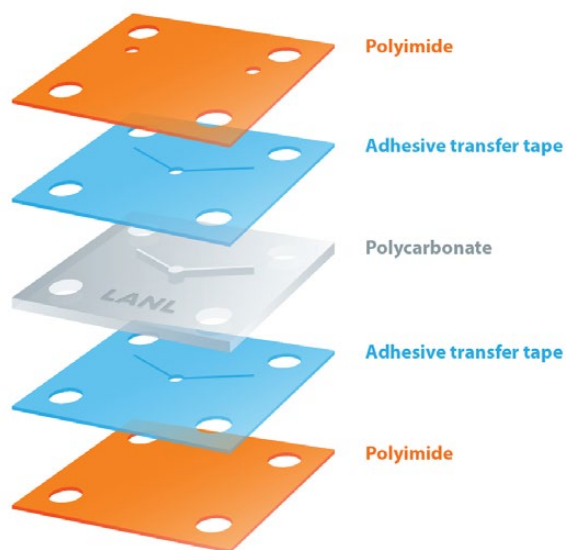


The logo for the Laboratory's Center for Integrated Nanotechnologies (CINT), etched into the surface of a human hair. The hair, which measures approximately 0.1 millimeters in diameter, was both donated and machined by scientist Quinn McCulloch as a droll demonstration of the capabilities of CINT's custom femtosecond laser.

Los Alamos earth scientists Hari Viswanathan and Bill Carey collaborate with McCulloch in their work studying geological fracture networks deep underground. Whether bringing material out of the ground (e.g., oil or gas) or putting material in to the ground (e.g., carbon dioxide or nuclear waste), fluid flow and transport occurring in subsurface fracture networks has to be well understood. Conditions at the surface aren't appropriate for modeling such phenomena—the temperature and pressure are too mild. Similarly, synthetic materials, though they may offer some advantages, are not as good as real rocks for understanding how real rocks behave. McCulloch makes microfluidic chips out of actual rock samples recovered from drilled cores, then Carey and Viswanathan load the chips with whatever fluid they're testing and place it into a special rig that applies heat and pressure comparable to 8000 feet below the earth's surface. Using real-time, high-resolution imaging, the scientists can evaluate where and to what extent the fluid travels through the microfluidic channels under such extreme conditions.

It's not practical to study fluid displacement in rocks 8000 feet below the surface of the earth. But with CINT's unique microfluidic capabilities, the exact conditions can be precisely replicated in the lab, bringing crucial light to an otherwise obscure natural system.





Cross-section diagram of a prototype device developed for conducting x-ray fluorescence spectroscopy, a method of elemental analysis, on small volumes of liquid spent nuclear fuel. The manufacturing method is lamination-based and uses layers of various materials.

## Radioactive recycling

Laboratories that handle actinides like uranium and plutonium are strictly limited in terms of the overall quantity of material that can be present in the facility at any given time. These materials are termed “materials at risk,” or MAR, and adherence to regulations, while paramount, also presents workflow challenges. Reducing the quantity of MAR needed for an experiment and the time needed to complete that experiment are therefore valuable advances that can streamline the workflow without compromising on safety. Los Alamos chemists Becky Chamberlin and Ning Xu have developed a way to reduce MAR quantity by up to 98 percent. And they did it with the help of microfluidics.

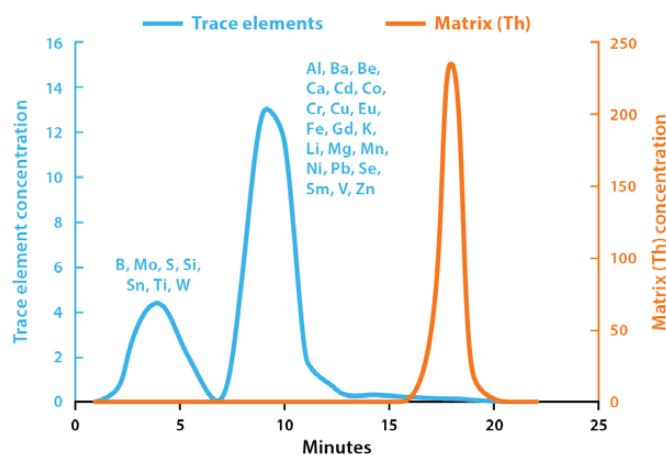
Plutonium is virtually nonexistent in nature, so it has to be manufactured, while uranium, though more abundant in nature, must be artificially enriched before it can be used industrially. During manufacture or recycling of these metals, it's important to know both the purity of the metal and the identity of any contaminating trace elements. The way this is usually done involves dissolving a small portion of the metal in a strong acid and then performing spectroscopy, which, in this case, identifies the elements in the sample by the wavelengths of light emitted when the atoms in the sample are excited by extreme heat. Unfortunately, plutonium emits light at a wide range of wavelengths, which can interfere with the identification and quantification of other elements in the sample. So the plutonium has to be separated out to allow the trace elements to be analyzed without that interference.

Chamberlin and Xu worked with Laboratory scientist Jun Gao to design a microfluidic device that efficiently separates plutonium from trace elements and which requires one-fiftieth the MAR quantity of traditional methods. The device incorporates resin microcolumns, through which the acid solution containing the dissolved metal sample is passed. The plutonium

atoms bind to the resin and are retained in the column while the trace elements in the solution pass through. Then, upon subsequent washing, the plutonium atoms are released into a separate fraction. At this point, the trace elements and the plutonium can be independently analyzed. This type of analysis is also useful for determining the history of smuggled nuclear material or materials of unknown provenance—an important task for national security.

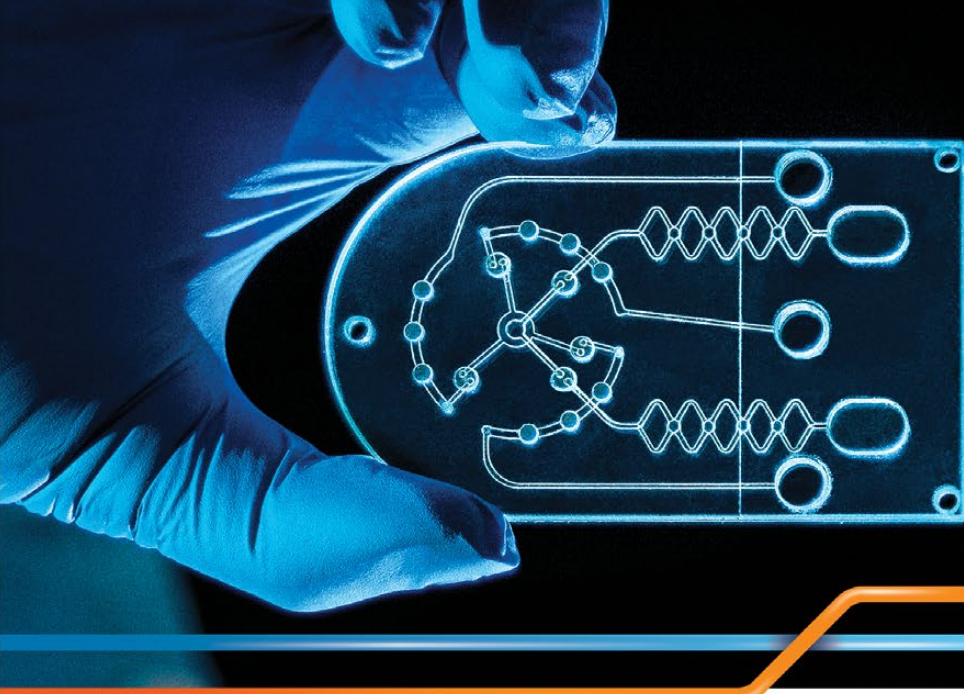
The microcolumn device uses a liquid-solid interface. But Chamberlin, with Los Alamos engineers Steve Yarbrow and Quinn McCulloch, has also created a liquid-liquid system to study fundamental plutonium chemistry. Similar in concept to the microdroplet system used by Starkenburg in his algal biofuels research, this device creates many uniform microdroplets of an organic phase (oil-like liquid) surrounded by an aqueous phase (water-based liquid). The interface between the two phases, located at the surface of the microdroplets, is where important chemistry happens—molecules within the aqueous phase react with molecules within the organic phase. By using microdroplets, the ratio of interface surface-area to volume is greatly increased, bringing more reactants from the two phases into contact and making the interface chemistry more efficient.

The microdroplet device has also been engineered to separate the two phases again after they've reacted with each other. By coating the inside of the microchannels, their surface properties can be prescribed in such a way that one channel is highly hydrophobic (water repelling) and the other is highly hydrophilic (water attracting). So the team's device neatly separates the mixture, shunting the aqueous phase down one channel and the organic phase down the other channel. Here too, as with the trace-element separation, the two phases can now be examined separately to learn about the chemistry that occurred at the microdroplet interface.



Plot showing the total separation of a metal sample into thorium (orange, right scale), an actinide element used initially in lieu of plutonium, and small quantities of contaminating trace elements (blue, left scale). The metal sample is dissolved into a liquid and passed through a resin column integrated within a microfluidic device. As the sample travels through the column, thorium atoms bind strongly to the resin, while certain trace elements pass immediately through (left blue peak) and others take slightly longer to pass through (center blue peak). After the trace-element sample is collected, a wash with a different solution releases the thorium atoms from the resin column (right orange peak).





Customizable microfluidic chip with incorporated pumps, valves, and mixer. The device has three inlets (large circles) and two outlets (large ovals). Any two of the three fluids from the inlets can be mixed by activating the incorporated pumps and valves (ring structure at left). The device is fast and affordable enough for one-time-use applications, and the pump can be customized to operate without electricity if needed, such as in a remote location.

### Onward flow!

Whereas logic in the general sense of sequential control systems is already guiding the design of Los Alamos microfluidic devices, logic in the strict sense is still coming along. But it's coming. The inclusion of automated if-then decision-making is the next phase for Nath and his collaborators. Integrating sensors that will measure temperature, color, or pH, for example, and take action based on those measurements, will bring Liquid Logic to the next level.

## A lofty vision for the future, personalized medicine carries enormous potential.

Nath has lofty visions for the future of Liquid Logic and microfluidics across Los Alamos. One relatively new project involves the integration of microfluidics with a nuclear magnetic resonance (NMR) platform for chemical-threat detection. This collaboration will combine two burgeoning Los Alamos capabilities: microfluidics and portable low-field NMR.

A goal for the immediate future is the further development of integrated functions. For example, McIntosh and Havrilla would like to include on their device the chemical separation steps of their spent nuclear-fuel measurement. This can be done with beads that selectively bind to certain ions, but it requires the addition of valves and pumps to orchestrate washing the beads. It also requires affordable mass production because the devices have to be disposable. Fortunately, once the engineering is done, the devices can be ultra-affordable, costing less than a dollar each when produced in large batches.

Another work in progress is the development of single-use devices with integrated features for applications in bioscience. The extraction of DNA or other molecules of biological interest from blood is a multistep process that can

benefit tremendously from being automated on microfluidic devices. These will require much smaller volumes of sample and reagents, as well as less time to completion, and, as with radioactive applications, must be single-use. But no matter, as, like the devices for actinide analysis, they can also be mass-produced for a very comfortable price tag.


The loftiest vision for the future, though in no way unrealistic, is personalized medicine and the enormous potential therein. If Liquid Logic devices like the ATHENA lung were to be available in doctors' offices or hospitals, each and every patient could be diagnosed and treated with laser precision. The disposable device would house the patient's own lung cells—not mouse cells or monkey cells—living and breathing as lung cells do. Drugs could be tested in each patient's unique physiology before deciding which drug should enter the patient's actual body. No more guesswork and no more waiting games. That wouldn't just be a good thing in a small package, it would be the very best thing in a small package. **LDRD**

—Eleanor Hutterer

### More on projects that use **microfluidics** at Los Alamos

- **Assessing the potential health hazards of nanotechnology**  
<http://www.lanl.gov/discover/publications/1663/2013-march/nanoparticle-toxicity-testing.php>
- **Chemical conversion of biomass for friendlier fuels**  
<http://www.lanl.gov/discover/publications/1663/2016-july/breaking-the-bond.php>  
<http://www.lanl.gov/discover/news-stories-archive/2016/February/acids-from-algae.php>
- **Ultra-low magnetic field technology**  
<http://www.lanl.gov/discover/publications/1663/2015-january/battlefield-mri.php>
- **New science to improve fuel-extraction in the United States**  
<http://www.lanl.gov/discover/publications/1663/2015-october/whats-lacking-with-fracking.php>  
<http://www.lanl.gov/discover/news-stories-archive/2015/June/supercritical-carbon-dioxide-fracturing-fluid.php>





# THE OTHER NUCLEAR REACTION

Neutron-capture reactions, responsible for the creation of most chemical elements, are being studied in detail for nuclear physics, nuclear technology, and national security.



IT'S NOT FISSION OR FUSION. It's not alpha, beta, or gamma decay, nor any other nuclear reaction normally discussed in an introductory physics textbook. Yet it is responsible for the existence of more than two thirds of the elements on the periodic table and is virtually ubiquitous anywhere nuclear reactions are taking place—in nuclear reactors, nuclear bombs, stellar cores, and supernova explosions.

It's neutron capture, in which a neutron merges with an atomic nucleus. And at first blush, it may even sound deserving of its relative obscurity, since neutrons are electrically neutral. For example, add a neutron to carbon's most common isotope, carbon-12, and you just get carbon-13. It's slightly heavier than carbon-12, but in terms of how it looks and behaves, the two are essentially identical. Add another neutron, however, and the story starts to get more interesting. Carbon-14 is radioactive with a 6000-year half-life. Carbon-15 and -16 are even more radioactive, decaying in mere seconds. Los Alamos nuclear scientist Shea Mosby, whose research is currently redefining human knowledge of key neutron-capture reactions, got his start doing graduate work on zeptosecond-lived carbon-21 (that's a billionth of a trillionth of a second).

"Nuclear power, nuclear weapons, nuclear medicine, and nuclear diagnostics—these things help to carry humanity forward, and neutron-induced reactions are vitally important to all of them," says Mosby. "So we strive to measure precise parameters for neutron capture by many different isotopes as part of the broader effort to understand all the ways to create and destroy every isotope of every element. And in nearly every isotope we've tested so far, we discovered something new and valuable."

## DANCE at LANSCE

At 30, Mosby is young for a Los Alamos staff scientist. His carbon-isotope research caught the attention of Lab scientist and now-colleague Aaron Couture during a recruiting trip to Mosby's graduate school. Couture hired Mosby as a postdoctoral researcher, broadening Mosby's experience with neutron capture to heavier elements, from iron to plutonium. Two years and 15 journal articles later, Mosby was given a permanent position.

Mosby's office and lab are located within the Los Alamos Neutron Science Center (LANSCE) complex, a proton accelerator facility that can be used to generate neutrons, which are siphoned off for his neutron-capture experiments. He wears a

dosimeter around his neck to track his exposure to radiation in the lab. And when he's not in the lab, he can keep tabs on his various experiments simultaneously from his office computer with not one or two but *five* widescreen monitors—displaying graphs and computer codes without a single pixel of unused space. Data printouts pinned to the wall on the left side of the office and techno-scribble densely covering the whiteboard on the right side testify to a man on a mission: developing, or at least contributing to, a detailed understanding of complex atomic nuclei. For that, he'll need to collect and tabulate a lot of cold, hard data.

Mosby's primary experimental apparatus for doing this is the Detector for Advanced Neutron Capture Experiments (DANCE), a heavily instrumented metal sphere with neutrons piped through the center, where they interact with a sample of the isotope being studied. Whenever neutrons enter the sample nuclei, they produce an excited nuclear state—essentially a high-energy arrangement of the protons and neutrons moving around in the nucleus. That high-energy state is unstable and proceeds to "relax" to the isotope's ground state, shedding its excess energy by emitting a series of gamma-ray photons. Those gamma rays enter a barium-fluoride scintillator array, where they kick electrons up to high speeds, energizing the material's crystal structure. The crystal then relaxes to its ground state by emitting ultraviolet photons, which are picked up by high-end optical detectors called photomultiplier tubes (PMTs), resulting in a measurable electrical signal. The scintillator array surrounds the sample, and the PMTs—which are extremely sensitive to ultraviolet but not to gamma rays—surround the scintillator array.

Once an experiment has been carried out, Mosby has to perform some calculations to obtain from DANCE's measurements a quantity known as the neutron-capture cross section—the proclivity for neutron capture of the type he measures to occur. From a practical standpoint, this single number encapsulates all useful information about that neutron capture by a given isotope. It is needed to understand and predict, for example, the mix of nuclear reactions that will take place inside a nuclear reactor, a weapon, or a star. It allows scientists to calculate the rate at which neutrons are lost to the reaction and the corresponding rate at which the resulting neutron-enriched nuclei do whatever they do next—whether that may be nuclear fission, radioactive decay, or capturing another neutron.



For example, in a typical nuclear power plant, neutrons bombard uranium-235 fuel. Several things can happen next. Ideally, the neutron induces a uranium atom to fission, splitting it in two and, in the process, spitting out a few more neutrons to interact with other uranium nuclei. Alternatively, the original neutron might enter the nucleus in such a way as to cause another neutron, or more than one, to reemerge. Or the neutron might be captured by the nucleus and excite (energize) it, causing a sequence of gamma rays to emerge. All of these processes have their own cross sections and affect the composition of the remaining neutron-and-fuel mixture and therefore the performance of the reactor. Different instruments measure the different cross sections for these processes; DANCE does its part by measuring the cross section for neutron capture leading to the emission of gamma rays.

## U and Pu

Before Mosby came to work at Los Alamos, some of his soon-to-be colleagues had set out to measure the neutron-capture cross section for uranium-235 and uranium-238, largely as a matter of course, to see if they could improve accuracy over previous measurements made with less sophisticated equipment. They did that, but interestingly, they also discovered something new based on DANCE's unique ability to resolve the many gamma rays involved in the nucleus's post-capture relaxation process.

It turned out that all prior calculations of the cross section as a function of neutron energy were greatly flawed: they predicted a spectrum of gamma rays very different from what

DANCE observed. The Laboratory's John Ullmann and others tracked down the discrepancy to a previously unknown set of transitions between nuclear states. Before this discovery, the calculated cross sections often differed from measurements by a factor of two at least—sometimes as much as ten! Now they're off by only 10 *percent*. With measurements this complex, that's a remarkable achievement. And because not all isotopes can be readily measured (some decay too quickly, others too violently), it is critically important to be able to reliably calculate the ones that can.

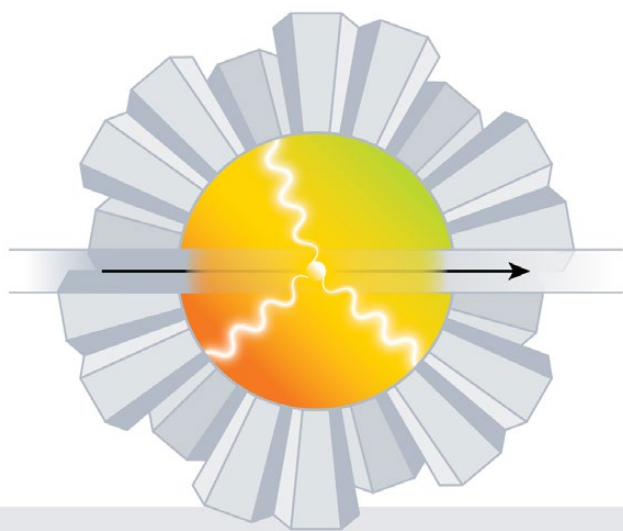
Mosby subsequently set out to measure the cross section for neutron capture onto plutonium-239, the primary fuel in a modern nuclear weapon. His results helped to resolve disputed cross-section estimates at the upper end of the relevant neutron-energy range. These results have been incorporated into the U.S. standard "evaluated nuclear data file" published by the National Nuclear Data Center (NNDC). This file is an important repository of nuclear data for use in a wide variety of nuclear technology applications.

According to Mosby, such updates are particularly important because some older NNDC data—particularly from the 1950s to 70s heyday of nuclear science and technology—suffers from inaccuracies caused by underestimated systemic uncertainties in the measurements made at the time. This can set back the field, delaying acceptance of updated values when new cross-section measurements are outside of the published uncertainty range because that range wasn't big enough to begin with, as was the case with the new plutonium-239 measurement at DANCE.

"It reminds me of the old saying, 'you have to be first, or right,'" says Mosby. "We're certainly in the business of doing it right, and we can't rely on earlier measurements for confirmation because those experimenters didn't have the decades of experience we have now. They didn't know all the things that can go wrong with a measurement like this, all the little gotchas. That means, for us, there is no answer key. We're writing the answer key."

In terms of Los Alamos's national security mission, getting that answer key right has two especially important uses. First, it is relevant for stockpile stewardship: maintaining the nation's nuclear deterrent largely with mathematical analysis instead of full-blown nuclear testing. That much reliance on calculations demands that all the input parameters be correct, including cross sections and a weapon's initial isotopic abundances. Fortunately, when it comes to maintaining the nation's own weapons, those initial abundances are known.

Second, the Lab is a specialist in nuclear diagnostics: analyzing a radioactive sample (such as the debris from a nuclear detonation) to reconstruct the details of how it was produced (the nature of the weapon and its nuclear material). In principle, this can be done by comparing the abundances of different isotopes present in the sample to determine what must have changed when the bomb went off. That only works if scientists have some way of knowing the initial abundances of certain isotopes (zero, for example, for isotopes produced solely by the weapon) and all the cross sections for

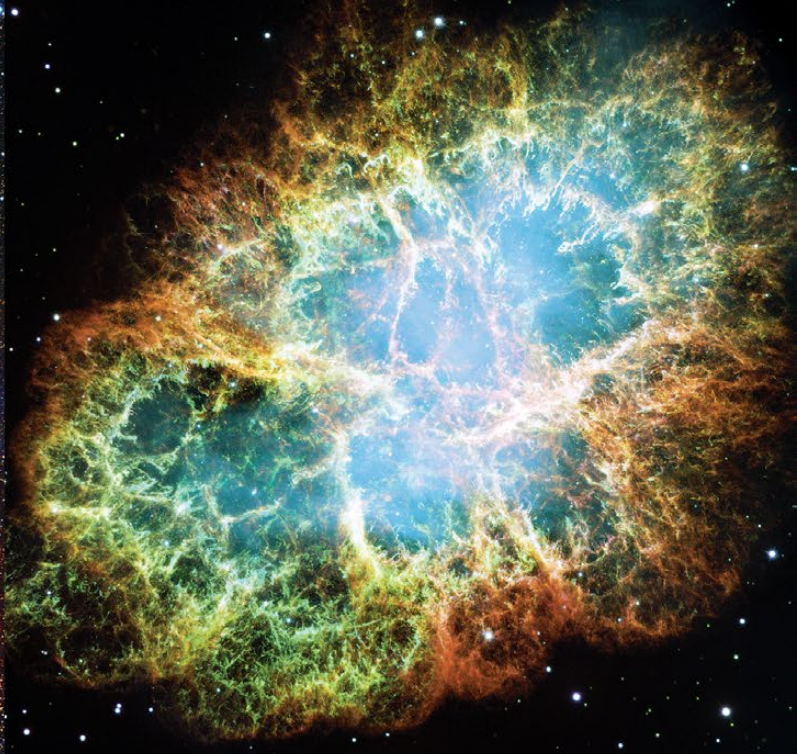


Neutrons pass through the DANCE detector and interact with an isotope sample at the center. Those neutrons that undergo neutron capture, entering a nucleus of the sample material, cause that nucleus to transition to a high-energy, excited state. The nucleus relaxes to its ground state by rapidly transitioning through a series of lower-energy states, emitting a gamma ray with each transition. Scintillators and detectors surrounding the sample obtain the energy and intensity of each gamma ray emitted.



When a star reaches old age, it swells to become a red giant; several are visible in this image of open star cluster NGC 3532. Some aging red giants, also known as asymptotic giants, host a number of neutron-producing reactions and, over time, produce heavier elements by successive neutron capture onto nuclei.

*CREDIT: (Left) ESO/G. Beccari; (Right) NASA, ESA, J. Hester, A. Loll (ASU)*



Massive stars, more than about ten times the mass of the sun, produce copious neutrons just before they go supernova, as do collisions between neutron stars, which are often left behind after such supernovae. Either event leads to an explosion that mashes nuclei and neutrons together, rapidly producing heavier elements by neutron capture. Shown here, the Crab Nebula, which harbors a neutron star near its center, is a supernova remnant.

every reaction that creates and destroys isotopes during the detonation. The more accurate the cross-section measurements are, the more sensitive the diagnostics will be.

### Dying stars

Mosby's answer key isn't only for bombs, power plants, and specialized nuclear physics labs. It's also integral to understanding the universe because neutron-capture reactions take place naturally in many astrophysical settings. These reactions are not only a point of academic interest to astronomers; they are also fundamental to the origin of most elements on Earth,

30 or so elements on the periodic table—elements like oxygen, silicon, and iron. (Hydrogen and helium are notable exceptions, having formed in abundance in the big bang.) But when stars reach old age, those fusion reactions become more complicated, with some producing free neutrons that are periodically captured by different nuclei present in the star. If the resulting nuclei are too neutron-rich to be stable, they will undergo beta decay, with a neutron turning into a proton (plus some other lighter particles), thus advancing the element by one position on the periodic table. (Elements are defined by atomic number, the number of protons in the nucleus.) Another neutron can then

## THE GOLD IN MY WEDDING BAND PROVES THERE ARE NEUTRON-CAPTURE REACTIONS IN THE UNIVERSE

including many that are important to industry (e.g., precious metals and medical isotopes) and a handful that are required for the human body to function (e.g., molybdenum in metabolic enzymes and iodine in thyroid hormones). Neutron-capture reactions are the primary source for most of these elements. As Mosby puts it, "Neutron-capture reactions underwrite our very existence."

For instance, stars generate much of their energy from a variety of nuclear-fusion reactions, which merge smaller elements into bigger ones and produce most of the first

be added, followed by another beta decay, thereby creating additional elements and moving across the periodic table. This is known as the slow, or s-process, one of two main varieties of astrophysical neutron capture.

The other occurs when massive stars die via supernova explosions or when neutron stars, frequent relics of such supernovae, collide with one another. Either event involves a blast of nuclei and neutrons, spawning a flurry of neutron-capture reactions known as the rapid, or r-process. The rapid, explosive addition of neutrons generally doesn't leave enough



time for beta decays to occur; as a result, many neutrons are crammed into each nucleus before there is a sufficient pause for a beta decay or two. Then more neutrons are slammed in before another beta decay occurs, and so on. Due to the neutron excess, r-process elements are highly radioactive, and only after the neutron infusion abates does a series of beta decays bring r-process elements back toward stability.

The s-process can produce elements up to bismuth, with atomic number 83; the r-process reaches uranium (92) and beyond. The r-process occurs in nuclear-weapon detonations as well. In fact, the last two elements that can be produced by the r-process, einsteinium (99) and fermium (100), were first discovered in the debris from the original hydrogen bomb detonation in 1952. Most heavy elements can be produced by both processes. Says Mosby, “The gold in my wedding band is proof of these neutron-capture reactions in the universe.”

Astrophysicists want to know how much of each element can be produced in each way in order to describe the chemical evolution of the universe. Mosby and colleagues have already experimented on some key branch points in the s- and r-processes. For example, they have discovered salient details in the process of neutron capture onto nickel-63. Nickel-63 beta decays to copper-63, which can capture another neutron and then beta decay to zinc-64. But DANCE results show that the cross section for neutron capture onto nickel-63 is substantially higher than previously thought, making it more likely to go to nickel-64 before decaying and therefore significantly reducing the production of copper-63 and zinc-64. Similarly, a DANCE study in collaboration with Louisiana State University updated neutron-capture cross sections for zinc-66, -67, and -68, which govern the likelihood of producing s-process isotopes up to rubidium, seven elements beyond zinc on the periodic table. Going forward, astrophysical models of element synthesis have to be modified to take these results into account.

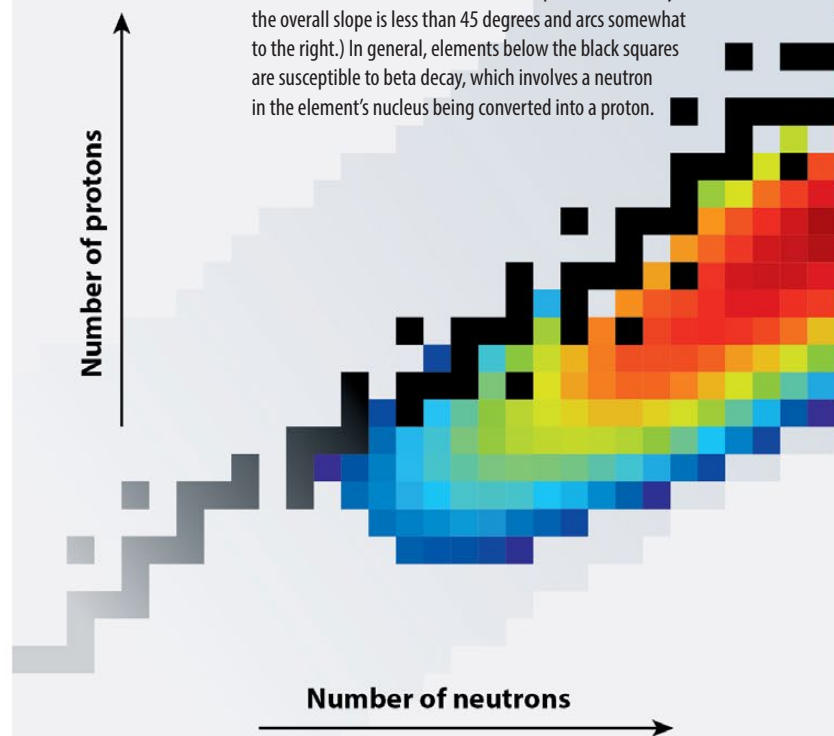
“I feel lucky,” says Mosby, “to be able to do research to advance nuclear technology and, at the same time, discover key details about how the universe works.”

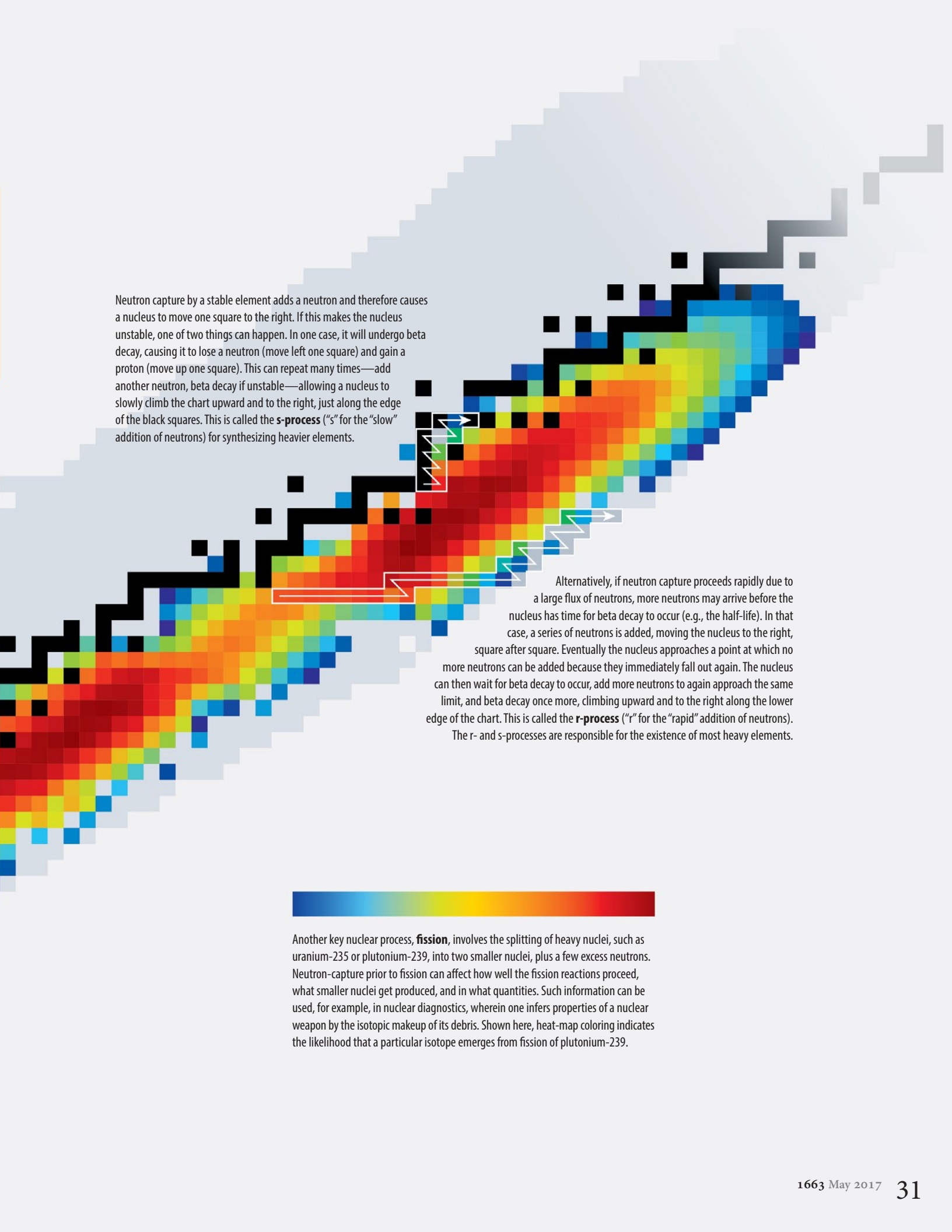
## The problem with prediction

DANCE is a highly sophisticated and successful experimental-physics machine. And yet, at its heart, it exists almost entirely for the purpose of covering up a hole in humanity’s ability to do nuclear physics: the ability to express the mathematical form of the strong nuclear force as it applies to all but the simplest nuclei. Physicists have well-established equations for the electromagnetic and gravitational forces, but they can’t perform an exact calculation to describe the force that confines protons and neutrons in an atomic nucleus (overpowering the repulsive electrical force among positively charged protons). As a result, physicists can’t predict from first principles the behavior, including interaction cross sections, for complex nuclei. Instead, they must measure these cross sections where possible and use the results to help estimate the properties of nuclei that have not been, or cannot be, measured.

**The chart of the nuclides**, a section of which is shown here, is the nuclear-physics equivalent of chemistry’s periodic table. The vertical axis counts the number of protons in a nucleus (which determines the element), and the horizontal axis counts the number of neutrons (which determines the isotope of that element). Each square on the chart represents a particular isotope of a particular element.

Black squares represent **stable isotopes**, but other squares are radioactive, usually because they deviate too far from an optimal proton-to-neutron ratio. (Because protons are positively charged and repel one another, a stable nucleus is more likely to stay stable with the addition of another neutron rather than another proton; that’s why the overall slope is less than 45 degrees and arcs somewhat to the right.) In general, elements below the black squares are susceptible to beta decay, which involves a neutron in the element’s nucleus being converted into a proton.





Neutron capture by a stable element adds a neutron and therefore causes a nucleus to move one square to the right. If this makes the nucleus unstable, one of two things can happen. In one case, it will undergo beta decay, causing it to lose a neutron (move left one square) and gain a proton (move up one square). This can repeat many times—add another neutron, beta decay if unstable—allowing a nucleus to slowly climb the chart upward and to the right, just along the edge of the black squares. This is called the **s-process** (“s” for the “slow” addition of neutrons) for synthesizing heavier elements.

Alternatively, if neutron capture proceeds rapidly due to a large flux of neutrons, more neutrons may arrive before the nucleus has time for beta decay to occur (e.g., the half-life). In that case, a series of neutrons is added, moving the nucleus to the right, square after square. Eventually the nucleus approaches a point at which no more neutrons can be added because they immediately fall out again. The nucleus can then wait for beta decay to occur, add more neutrons to again approach the same limit, and beta decay once more, climbing upward and to the right along the lower edge of the chart. This is called the **r-process** (“r” for the “rapid” addition of neutrons). The r- and s-processes are responsible for the existence of most heavy elements.

Another key nuclear process, **fission**, involves the splitting of heavy nuclei, such as uranium-235 or plutonium-239, into two smaller nuclei, plus a few excess neutrons. Neutron-capture prior to fission can affect how well the fission reactions proceed, what smaller nuclei get produced, and in what quantities. Such information can be used, for example, in nuclear diagnostics, wherein one infers properties of a nuclear weapon by the isotopic makeup of its debris. Shown here, heat-map coloring indicates the likelihood that a particular isotope emerges from fission of plutonium-239.





The DANCE neutron-capture experiment.

CREDIT: Robb Kramer/LANL

Even the act of comparing measurements to theory is frustratingly inexact. Mosby seeks to measure the cross section for neutron capture resulting in the emission of gamma rays. But what he actually measures is the distribution of emitted

## I GET TO ADVANCE NUCLEAR TECHNOLOGY AND DISCOVER KEY DETAILS ABOUT HOW THE UNIVERSE WORKS

gamma rays after neutron capture, which theoretically depends on the particular nuclear structure of the isotope being investigated. In order for his measurements to translate into the ability to predict other isotopes' cross sections, he must develop a reliable mathematical relationship that links the isotope's nuclear structure, its gamma-ray emissions following neutron capture, and its cross section.

Unfortunately, for most isotopes, the gamma-ray emissions are far too complicated to be predicted mathematically. When a neutron is absorbed, it deforms the nucleus somewhat, sending that nucleus into the highly excited state that relaxes by emitting gamma rays. But there can be thousands of intermediate states between this excited state and the ground state,

meaning that thousands of gamma rays of different energies are emitted along the way. It's too computationally intensive to calculate directly. So instead, Mosby, like others in the field, is forced to work with an approximation, a complicated average across all the gamma-ray energies known as the photon strength function (PSF). It's not ideal, but it's the best he can do. He uses DANCE measurements of gamma rays to calibrate estimated PSFs, and works in two directions from there. In the theoretical direction, he uses gamma-ray measurements to reveal the properties of the isotope's intrinsic nuclear structure. And in the practical direction, he uses an established formula—albeit a messy one—to arrive at the cross section needed for nuclear science and technology applications.

Not all isotopes are created equal for this kind of work. Mosby recently tried an experimental series on the isotope zirconium-96 because it happens to have an unusually small number of nuclear transitions—at least compared to actinide elements like uranium and plutonium that DANCE often studied in the past—between its ground state and the various states excited by neutron capture. Here, the averaging built into the PSF starts to break down because there aren't enough different gamma-ray producing transitions to develop a meaningful average. In one sense, that makes zirconium-96 a particularly clean isotope for study, in that it might allow a simpler-than-usual connection between nuclear structure, neutron-induced deformation of the nucleus, the PSF, and the cross section. The results may help identify and correct the flaws in neutron-capture cross sections across the board.

For Mosby's part, he is interested in a holistic treatment of the problem, pushing the limits of the PSF—an artificial construct—to get at the underlying reality of the available nuclear states. Measure some isotopes. Learn to calculate others. Work backwards to better understand nuclear physics, and tabulate cross sections for nuclear power, medicine, weapons, diagnostics, astrophysics, and other applications yet to be discovered. Along the way, he savors being able to make tangible progress every time he throws a neutron at a new isotope. **LDRD**

—Craig Tyler

### More nuclear physics applications at Los Alamos

- **Nuclear fusion power research**  
<http://www.lanl.gov/discover/publications/1663/2016-july/small-fusion-could-be-huge.php>
- **Subcritical nuclear weapons experiments**  
<http://www.lanl.gov/discover/publications/1663/2014-august/critical-subcritical.php>
- **Nuclear medicine**  
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- **Nuclear astrophysics**  
<http://www.lanl.gov/discover/news-release-archive/2016/April/04.21-burst-code-probes%20.php>  
(See also page 2 of this issue of 1663.)
- **Entombing nuclear waste**  
<http://www.lanl.gov/discover/publications/1663/2013-march/disposing-nuclear-waste-in-salt-bed%20.php>





Camouflage in nature is frequent and exquisite, as demonstrated in this watercolor painting entitled "Male Ruffed Grouse in the Forest" by Gerald Thayer. Thayer and his father, Abbott Thayer, were naturalists and artists whose 1909 collaborative book, "Concealing Coloration in the Animal Kingdom," is thought to have influenced the adaptation and evolution of camouflage in the military. Los Alamos scientists are using animals' camouflage to develop computer algorithms that automatically detect hidden objects in photographs. For more on defeating camouflage, see "Beating the Best Camouflage" on page 3.

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The Sangre de Cristo mountain range, running from central Colorado to just southeast of Santa Fe, New Mexico, forms the southernmost extent of the Rocky Mountains.

*CREDIT: Elena E. Giorgi*



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